

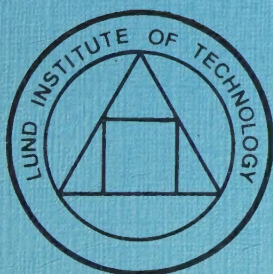
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*THEORETICAL AND EXPERIMENTAL INVESTIGATIONS
OF
ATOMIC STRUCTURES AND LIFETIMES*

BY

CLAES-GÖRAN WAHLSTRÖM

LRAP-67



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*LUND INSTITUTE OF TECHNOLOGY
OCTOBER 1986*

<i>CONTENTS</i>	page
ABSTRACT	2
LIST OF PAPERS	3
1 INTRODUCTION	4
2 THE THEORY OF ATOMIC STRUCTURE AND RADIATIVE PROPERTIES	6
3 EXPERIMENTAL TECHNIQUES	13
3.1 Energy level system	13
3.2 Hyperfine structure	15
3.3 Radiative lifetimes	19
4 THEORETICAL METHODS	22
4.1 The central field model	23
4.2 The variational principle	25
4.3 The Hartree-Fock method	26
4.4 Energy matrix diagonalization and parametric fits to energy levels	28
4.5 Brillouin's theorem	30
4.6 Configuration-interaction methods Multi-configuration Hartree-Fock	31
4.7 Effective operators and perturbation theory	33
4.7a Effective hyperfine operators	33
4.7b Many-body perturbation theory	34
4.8 The Coulomb approximation	40
5 COMMENTS ON THE PAPERS	42
6 ACKNOWLEDGEMENTS	45
7 REFERENCES	46
8 PAPERS	50

*Do not follow where the path may lead,
Go, instead, where there is no path
and leave a trail.*

ABSTRACT

Theoretical and experimental investigations of the energy level structure of Sr^{++} , Rb^{3+} and Xe^{2+} , hyperfine structures of excited states in neutral Al, Ga and In and radiative lifetimes of a number of states in Ga and Sr are reported on in this thesis. The different experimental techniques and theoretical methods used are presented and compared.

The SrV, RbIV and XeIII spectra were recorded photographically and the observed level structures interpreted by means of Hartree-Fock calculations and parametric fits. Rydberg-series configuration interactions were included in the theoretical interpretation and their effects on the level structures investigated. It was found that $p^3nd \leftrightarrow p^3n'd$ configuration interactions play an important role in the determination of the 3S term in p^3d configurations.

The XeIII analysis includes an interpretation of the Xe $N_{4,5}00$ Auger spectrum, and the spectral lines classified include most of the observed XeIII laser lines.

Hyperfine structures were measured using tunable single-mode dye-lasers and collimated atomic beams, or using pulsed lasers and the quantum beat technique. The observed structures were interpreted by semi-empirical methods or compared with theoretical *ab initio* values. The theoretical calculations were performed using Many-Body Perturbation Theory, including core polarization to all orders and electron correlation in the lowest order, or using the Multi-Configuration Hartree-Fock method.

Radiative lifetimes were investigated experimentally by studying the fluorescence light after selective laser excitation. Transient recordings as well as delayed coincidence methods were utilized. Theoretical *ab initio* lifetimes have been calculated using the Multi-Configuration Hartree-Fock method. The radiative lifetimes of excited states in the Ga $4s^2nd\ ^2D$ series are found to be strongly affected by the non-localized $4s4p^2\ ^2D$ perturber. Severe cancellation is observed in certain transition probabilities, theoretically as well as experimentally.

The effect of hyperfine-induced singlet-triplet mixing on the radiative lifetimes has been studied in neutral Sr. Different lifetimes were, for the first time, using laser spectroscopic measurements combining high spectral and temporal resolution, observed for different hyperfine components. The experimental results are in good agreement with theoretical calculations.

LIST OF PAPERS

This thesis is based on the following papers:

- I. W. Persson and C.-G. Wahlström, Spectrum of Sr V, *Physica Scripta* **30**, 169 (1984).
- II. W. Persson and C.-G. Wahlström, Spectrum of Rb IV, *Physica Scripta* **31**, 487 (1985).
- III. W. Persson, C.-G. Wahlström, G. Bertuccelli, H.O. DiRocco, J.G. Reyna Almandos and M. Gallardo, Revised and extended analysis of Xe III, Preliminary manuscript.
- IV. G. Jönsson, C. Levinson, S. Svanberg and C.-G. Wahlström, Natural radiative lifetimes and hyperfine structure of the $4s^2 6p^2 P_{3/2,1/2}$ levels of gallium, *Phys. Lett.* **93A**, 121 (1983).
- V. G. Jönsson, C. Levinson, I. Lindgren, A. Persson and C.-G. Wahlström, Experimental and theoretical studies in the $4s^2 np^2 P$ sequence of neutral gallium, *Z. Phys. A: Atoms and Nuclei* **322**, 351 (1985).
- VI. Y.-Y. Zhao, J. Carlsson, H. Lundberg and C.-G. Wahlström, Hyperfine structure studies in 2D and 4P states of ^{27}Al , $^{69,71}Ga$ and ^{115}In . Accepted for publication in *Z. Phys. D*.
- VII. H. Bergström, C. Levinson, H. Lundberg, S. Svanberg, C.-G. Wahlström and Zhao You Yuan, Hyperfine-dependent lifetimes induced by singlet-triplet mixing, *Phys. Rev. A* **33**, 2387 (1986).
- VIII. G. Jönsson, C. Levinson, A. Persson and C.-G. Wahlström, Natural radiative lifetimes in the 1P_1 and 1F_3 sequences of Sr I, *Z. Phys.* **A316**, 255 (1984).
- IX. J. Carlsson, H. Lundberg, W.X. Peng, A. Persson, C.-G. Wahlström, T. Brage and C. Froese Fischer, Experimental and theoretical investigation of radiative lifetimes in neutral gallium. Accepted for publication in *Z. Phys. D*.
- X. T. Brage, C. Froese Fischer, J. Carlsson and C.-G. Wahlström, Lifetimes and oscillator strength trends for the $4s^2 nd^2 D$ series of Ga I. Accepted for publication in *Phys. Rev. A*.

1 INTRODUCTION

The subject of this thesis is the investigation of some fundamental atomic interactions and properties. To study the physical interactions which exist within an atom or ion, one must study how it interacts with its surroundings, or investigate the light emitted from excited atoms. (In the following I will write "*atom*", but the word can equally well be read as "*ion*".)

A free atom consisting of N electrons, each of charge $-e$ and a positive nucleus of charge Ze constitutes a bound physical system with certain well defined energy eigenstates. When such a free atom makes a transition from a state with high energy to a state with lower energy, the energy difference is emitted as a photon. The frequency ν of the emitted photon is related to the energy difference ΔE between the two states involved by the relation $\Delta E = h\nu$, where h is Planck's constant. The inverse process, absorption of a photon is also possible if the energy of the incoming photon matches an energy separation between the initial state of the atom and some excited state.

By obtaining the spectra of emitted or absorbed light, however, we can only ascertain the existing energy separations. Theoretical models and systematic methods are then required to deduce the energies of the individual atomic states - the energy level system. The energy levels and transition probabilities reflect the different physical interactions which occur within the atoms (and possibly with surrounding electric and magnetic fields).

By constructing theoretical models for the atoms and the different forms of interactions occurring, attempts are made to reproduce the experimental energy level structures and the observed radiative properties. In this way, new knowledge about the system under study and a deeper understanding about atomic interactions can be obtained. The size and relative importance of the different kinds of interactions can be clarified. Sometimes the model used has to be extended and improved to explain the structures and properties found experimentally. Using the knowledge and models obtained, new predictions can be made. Sometimes peculiar effects or deviations from the "normal" behaviour can be predicted, and new interesting experiments can be arranged to investigate these effects.

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In 1980, Sune Svanberg was installed as Professor of Atomic Physics at the Lund Institute of Technology. The main activities were then directed towards laser spectroscopy and related applications, but with the work on emission spectroscopy of ions remaining. The research group has been growing constantly since then, in the number of active researchers and students, as well as in the amount of results obtained.

The basic atomic physics group did, however, suffer from a lack of theoretical activity supporting the experimental work. At Chalmers Institute of Technology in Gothenburg, where professor Svanberg and several of the graduate students came from, there existed a good balance between experimental and theoretical activities within the research group.

The assignment for my graduate work, when I started in the group in 1982, was to initiate some theoretical activity within the Lund group. The object of this was, in particular, to perform theoretical calculations supporting the experimental work. It was believed that the experimental work would be even more fruitful through theoretical analyses of the results obtained, especially when they differed significantly from the "expected". It was also hoped that theoretical predictions would guide the experimental activity to interesting fields. Another objective was to establish contacts and to initiate collaborations with theoretical groups at other laboratories.

By working part of the time with experiments, learning about lasers, experimental methods, and, in particular, about different practical limitations, an immediate connection between the different activities was aimed for. The majority of my time has, however, been devoted to the theoretical programme.

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The lay-out of this thesis is as follows. After this introductory section on the motivations for theoretical activities in an experimental research group, a brief outline of the physical interactions present in atoms or ions is presented. The origin of e.g. the gross, fine and hyperfine structures will be discussed, and the effect of external electric and magnetic fields giving rise to Zeeman and Stark effects will also be mentioned. At the end of that chapter some radiative properties of atoms are presented.

In the next chapter, some experimental methods are presented together with some of their limitations and sources of errors. A number of methods will be mentioned, even if only briefly. This is done to place the methods used in the work presented in this thesis in a larger context. The subjects presented in this chapter range from different light sources and spectrographs used in emission spectroscopy to various high-resolution laser spectroscopic techniques used for hyperfine structure measurements, and on to beam-foil and time-resolved laser techniques used for lifetime measurements.

The following chapter is devoted to a presentation and comparison of different theoretical methods - or approaches. Energy-matrix diagonalization and parametric least-squares fitting methods for the interpretation of gross and fine energy structures are described. Variational methods, such as Hartree-Fock (HF) and Multi-configuration Hartree-Fock (MCHF) are compared. Effective hyperfine operators and the diagrammatic form of many-body perturbation theory (MBPT) are outlined.

In the last chapter, finally, some comments on the different papers are made.

2 ATOMIC STRUCTURES AND RADIATIVE PROPERTIES

The most complete description that can be given of an atom in a specific state is by the quantum mechanical wavefunction Ψ . To obtain this wavefunction for a stationary state, we must solve the *Schrödinger equation*, which can be written as

$$H\Psi^{(i)} = E^{(i)}\Psi^{(i)} \quad (i=1,2,3\dots) \quad (2.1)$$

Here H is the *Hamiltonian* of the system and $\Psi^{(i)}$ is the wavefunction for the i^{th} state having the energy eigenvalue $E^{(i)}$. (In a fully relativistic treatment the relativistic Dirac equation [1] should instead be solved. In this thesis, however, mainly non-relativistic atomic theory will be discussed.) The theoretical challenge is therefore twofold. First the quantum mechanical Hamiltonian must be formed, taking the different atomic energy contributions into account; then the Schrödinger equation must be solved. In this section the Hamiltonian is constructed, and some operators for the calculation of transition probabilities are presented. The task of solving the equation is treated in chapter 4.

GROSS ENERGY STRUCTURE

The dominant contributions to the energy of an atom are the kinetic energy of the electrons, the attractive electrostatic Coulomb force between each electron and the nucleus and the repulsive Coulomb force acting between the electrons. These interactions are included in the total energy by including the terms

$$\begin{aligned} H_{\text{kin}} + H_{\text{electron-nucleus}} + H_{\text{electron-electron}} = \\ = -\frac{1}{2} \sum_i \nabla_i^2 - \sum_i \frac{Z}{r_i} + \sum_{i>j} \frac{1}{r_{ij}} \end{aligned} \quad (2.2)$$

in the total *non-relativistic* Hamiltonian for the atom.

The summations are carried out over all the electrons and over all pairs of electrons, r_i is the distance between electron i and the nucleus, and r_{ij} is the distance between the i^{th} and j^{th} electrons. (Unless specified otherwise Hartree atomic units [2] are used. The basic units are the rest mass of the electron $m=1$, the absolute value of the charge of the electron $e=1$, $\hbar/2\pi=1$ where $\hbar$ is Planck's constant and $4\pi\epsilon_0=1$ where ϵ_0 is the permittivity of vacuum. With these basic units the unit of length is the first Bohr radius, a_0 , the unit for energy the Hartree atomic unit, H ($1H=2Ry$), and $\mu_0/4\pi=\alpha^2$ where μ_0 is the permeability of vacuum and α the fine-structure constant.)

These contributions to the total Hamiltonian give rise to the gross energy structure of the atom. The configurations are formed and the energies of these are split into different LS terms.

FINE STRUCTURE

To include more interactions in the Hamiltonian we turn to some magnetic interactions of a relativistic nature. These involve the intrinsic spin of the electrons. Some of these interactions give rise to energy splittings of the LS terms, resulting in different energies depending on the total angular momentum, J , of the atomic electrons. This is the *fine structure* in the atomic energy level system.

The orbital motion of electron i in the electric field $\mathbf{E}_i$, produced by the nucleus and the other electrons, gives rise to, in the rest frame of the electron, a magnetic field which interacts with its spin, $\mathbf{s}_i$. A quantum mechanical treatment based on the relativistic Dirac equation leads to the operator [3]

$$\begin{aligned} H_{\text{spin-orbit}} &= \frac{\alpha^2}{2} \sum_i (\mathbf{E}_i \times \mathbf{p}_i) \cdot \mathbf{s}_i = \\ &= \frac{\alpha^2}{2} \left(\sum_i \frac{Z}{r_i^3} \mathbf{r}_i \times \mathbf{p}_i - \sum_{j \neq i} \frac{\mathbf{r}_{ij}}{r_{ij}^3} \times \mathbf{p}_i \right) \cdot \mathbf{s}_i. \end{aligned} \quad (2.3)$$

This is called the *spin-(own)-orbit* interaction ($\mathbf{r}_i \times \mathbf{p}_i$ is sometimes written as $\mathbf{l}_i$). There is also the *spin-other-orbit* interaction, originating from the interactions between the spin of electron j and the magnetic field produced by the orbital motion of another electron i . This interaction can be added to the Hamiltonian by the operator

$$H_{\text{spin-other-orbit}} = \alpha^2 \sum_{ij} \left(\mathbf{p}_i \times \frac{\mathbf{r}_{ij}}{r_{ij}^3} \right) \cdot \mathbf{s}_j. \quad (2.4)$$

In addition to these there are other magnetic interactions in many-electron systems which can be interpreted as spin-spin and orbit-orbit interactions. These effects, however, are very small and can normally be neglected.

When using the central field model of the atom, which will be described later, it is possible to make important simplifications in the treatment of the magnetic interactions. An "effective" one-body operator is introduced

$$H_{\text{spin-orbit}}^{\text{eff}} = \sum_i \zeta_i \mathbf{l}_i \cdot \mathbf{s}_i \quad (2.5)$$

where the summation runs over the open shells only. The parameter ζ_i is called the *spin-orbit parameter*, but it should be observed that it can be defined to contain most of the spin-other-orbit interaction as well. In a local, central potential u - neglecting the spin-other-orbit interactions, the spin-orbit parameter above simply reduces [4] to the expression

$$\zeta = \frac{\alpha^2}{2} \left\langle \frac{1}{r} \frac{du}{dr} \right\rangle \quad (2.6)$$

where $\langle \rangle$ represents the expectation value in the open shell.

By using only these first four terms in the total Hamiltonian and treating the spin-(own)-orbit and some of the spin-other-orbit by the effective spin-orbit operator (2.5) we have

$$-\frac{1}{2} \sum_i \nabla_i^2 - \sum_i \frac{Z}{r_i} + \sum_{i>j} \frac{1}{r_{ij}} + \sum_i \zeta_i \mathbf{l}_i \cdot \mathbf{s}_i \quad (2.7)$$

This Hamiltonian represents the gross and fine energy structure of an isolated atom or ion. In papers I, II and III these structures in Sr^{++} , Rb^{3+} and Xe^{2+} are studied experimentally and interpreted theoretically using the above Hamiltonian.

HYPERFINE STRUCTURE

The next kind of interactions which have to be included to obtain a more complete picture of the atom and its energy level structure are the so-called *hyperfine interactions* (hfi) giving rise to the *atomic hyperfine structure* (hfs). These interactions occur only if the atomic nucleus possesses an intrinsic spin, $\mathbf{I}$, and may be different for different isotopes.

The origin of the hfi lies in the fact that a nucleus with non-zero nuclear spin $\mathbf{I}$, not only acts as a positively charged point - an electric monopole, but it also has electromagnetic multipole moments of higher orders. The interactions between these moments and the electromagnetic field at the nucleus, produced by the electrons, create additional energy contributions depending on the total angular momentum of the atom

$$\mathbf{F} = \mathbf{I} + \mathbf{J} \quad (2.8)$$

(If the angular momentum $\mathbf{J}$ of the electrons is zero, there may be a small *shift*, but obviously no hyperfine *splittings*.)

Generally, we can express the hyperfine operator in terms of scalar products of electronic ($\mathbf{T}^k$) and nuclear ($\mathbf{M}^k$) tensor operators [5]

$$H_{\text{hfi}} = \sum_{k=1}^{\infty} \mathbf{T}^k \cdot \mathbf{M}^k. \quad (2.9)$$

$\mathbf{M}^k$ represents the 2^k -pole moments of the nucleus and $\mathbf{T}^k$ the corresponding field at the site of the nucleus. For parity reasons, magnetic interactions contribute only for odd k (dipole, octupole, etc) and electric interactions only for even k (monopole, quadrupole, hexadecapole etc). $\mathbf{T}^k$ is the sum of one-body operators, and we can write it as a summation over all the individual electrons

$$\mathbf{T}^k = \sum_i \mathbf{t}_i^k. \quad (2.10)$$

The two most important moments, besides the strongly dominant electric monopole already considered, are the magnetic dipole and electric quadrupole moments.

The magnetic dipole interaction can be added to the Hamiltonian through the operator [5]

$$H_{\text{hfi-dipole}} = \alpha^2 \sum_i (\mathbf{l}_i r^{-3} - \sqrt{10} (\mathbf{s} \mathbf{C}^2)^1 r^{-3} + \frac{8\pi}{3} \mathbf{s} \delta(\mathbf{r})) \mu_I. \quad (2.11)$$

Here $\mathbf{l}$ and $\mathbf{s}$ are the orbital and spin angular momentum operators, respectively, of the i^{th} electron, $(\mathbf{s}\mathbf{C}^2)^1$ is a tensor product of $\mathbf{s}$ and $\mathbf{C}^2$ of rank 1 ($\mathbf{C}^2$ is a renormalized spherical harmonic) and $\delta(\mathbf{r})$ is a three-dimensional delta function. μ_I is the nuclear magnetic moment.

The electronic part, given by the sum of the terms within the large brackets, represents the magnetic field at the site of the nucleus due to the electrons. The first term is caused by the orbital motion of the electrons, and is called the *orbital* term. The second term represents the dipole field due to the spin motion of the electrons and is called the *spin-dipole* term. These two terms, which have an r^{-3} radial dependence, contribute only for non-s electrons. The last term of the dipole operator represents the *contact interaction* between the nucleus and the electron spin, and contributes only for s-electrons.

The interaction between the electric quadrupole moment of the nucleus and the electric field gradient at the site of the nucleus produced by the electrons, can be represented by the operator [5]

$$H_{\text{hfi-quadrupole}} = -\frac{1}{2} \sum_i \mathbf{C}^2 \mathbf{Q}^2 r^{-3} \quad (2.12)$$

where $\mathbf{Q}$ is the nuclear electric quadrupole tensor.

It can be shown that, when only matrix elements diagonal with respect to J are considered, the resulting energy contributions from the magnetic dipole and electric quadrupole interactions can be expressed as

$$\begin{aligned} \Delta E_{\text{hfs}} &= \Delta E_{\text{dipole}} + \Delta E_{\text{quadrupole}} = \\ &= \frac{1}{2} A(J)C + B(J) \frac{3/2 C(C+1) - 2J(J+1)I(I+1)}{2J(2J-1)2I(2I-1)} \end{aligned} \quad (2.13)$$

where

$$C = F(F+1) - J(J+1) - I(I+1)$$

and A and B are the hyperfine coupling constants for the dipole and quadrupole interactions, respectively.

Using different experimental and theoretical methods, hyperfine structures in neutral Al, Ga and In are studied and presented in papers IV, V and VI. The results from these experimental investigations are presented as A and B factors. Theoretical calculations of the A and B factors, for comparisons between experiment and theory, were performed using the operators (2.11) and (2.12). A remarkable influence of the hyperfine interactions on the radiative lifetimes of some high-lying states in neutral Sr is reported on in paper VII.

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So far only interactions within an isolated atom (or ion) have been considered. If external electric or magnetic fields are present further terms have to be added to the Hamiltonian.

INTERACTIONS WITH STATIC EXTERNAL FIELDS

The interaction of the atomic magnetic moment $\mu_I + \mu_J$ and an external magnetic field $\mathbf{B}_{\text{ext}}$ gives rise to, e.g., the *Zeeman effect* [6]. This effect manifests itself by splitting different fine and hyperfine structure levels into magnetic sublevels. The interaction can be expressed by the operator

$$H_{\text{magn}} = -\mu_I \cdot \mathbf{B}_{\text{ext}} - \mu_J \cdot \mathbf{B}_{\text{ext}} \quad (2.14)$$

where the first term only exists if the atomic nucleus possesses a nuclear magnetic moment. Even then it is normally much smaller than the second term and can be neglected. These additional energies depend on the strength of the external magnetic field.

In the case of weak magnetic fields, the observed energy contributions can be expressed as

$$\Delta E_{\text{magn}} = g_J \mu_B M_J B_{\text{ext}} \quad (2.15)$$

where g_J is known as the Landé g -factor. The value of the g_J factor reflects the coupling conditions of the angular momenta in the atoms, and it is therefore of interest to compare experimental and theoretical values. The qualitative form of the contribution of the magnetic field to the level structure is, however, independent of the coupling conditions: each zero-field level is broken up into a set of $2J + 1$ equally spaced sublevels, symmetrically arranged about the zero-field position; M_J increases from $-J$ for the lowest sublevel to $+J$ for the highest (for positive g_J).

If the atom is placed in an external electric field, $\mathbf{E}_{\text{ext}}$, there is an additional term in the Hamiltonian

$$H_E = -\sum (-e\mathbf{r}_i) \cdot \mathbf{E}_{\text{ext}}. \quad (2.16)$$

This interaction gives rise to the *Stark effect* [7] which can shift as well as split energy levels.

The influence on the energy levels of external electric and magnetic fields has not been investigated experimentally in any of the papers presented in this thesis. However, when performing some of the lifetime measurements experimental precautions had to be taken to avoid the influence of small Zeeman splittings due to the earth's magnetic field. In the work on Xe^{2+} theoretical g_J factors were calculated and compared with experimental g_J factors existing in the literature for some of the states.

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If now the eigenvalue problem (2.1) could be solved

$$H_{\text{tot}} \Psi^{(i)} = E^{(i)} \Psi^{(i)} \quad (i=1,2,3,\dots)$$

with all the terms described above included in the total Hamiltonian, the entire energy structure of the atom would be known. The theoretical work would be completed. (Most of the relativistic effects and some other smaller effects have, however, not been included.)

The big problem, however, is that it is impossible to solve the Schrödinger equation analytically for many-electron atoms. Even using numerical methods and fast computers, the task is, in practice, impossible. Several simplifications to the total Hamiltonian must therefore be made. This partly explains why the different papers in this thesis each treat only certain specific effects and why so many different theoretical methods are required. By making estimates concerning the relative importance of the different terms, the most important ones, for the effect under study, can be selected and the rest omitted. Many of the smaller effects can then be evaluated separately with varying accuracy by different perturbation methods.

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The discussion has, so far, been limited to the energy eigenvalues of the atoms. It is also important to know the probability of transitions between states of different energies, and these are therefore also studied.

RADIATIVE PROPERTIES

An atom, or ion, always wants to be in its lowest possible energy eigenstate, the ground state. By adding energy to the system, either by irradiation with light or collisions with e.g. other atoms, ions or electrons, the atom may be excited to an eigenstate of higher energy. After populating a specific excited state, i , the atom has a spontaneous emission transition probability, A_{if} per unit time of making a transition to any state f of lower energy. During such a transition the atom emits a photon of frequency

$$\nu_{if} = (E_i - E_f)/h. \quad (2.17)$$

The time taken, on average, after exciting N_0 atoms into the energy eigenstate, i , until only N_0/e atoms remain in this state, is the *natural radiative lifetime*, τ , of that state.

$$\tau_i = 1 / \sum_f A_{if} \quad (2.18)$$

where the summation is over all levels, f , with energies less than E_i .

In some cases it is of fundamental interest to study the radiative lifetimes of excited atomic states. This is the case e.g. in the search for possible new laser media and laser transitions. In other cases the main interest lies in knowing the individual transition probabilities. Through knowing the transition probabilities, A_{if} or the closely related oscillator strengths f_{if} , important information about the atoms and their surroundings can be obtained. By recording and comparing the strengths of individual spectral lines in the light from distant stars or from laboratory fusion experiments, not only chemical compositions, but also e.g. the temperatures and densities can be deduced. If the lifetime is not infinite, the Heisenberg uncertainty principle implies a finite width, $\delta E = h/2\pi\tau$, of the energy level i and a corresponding natural width, $\delta\nu$, of the spectral lines. Therefore, by knowing the radiative lifetimes of atomic states, the ultimate resolution limits for energy level determinations are also known.

To calculate accurate *ab initio* transition probabilities (and lifetimes) would not be difficult if the Schrödinger equation with the full Hamiltonian could be solved exactly. Not only would all the energy eigenvalues be obtained, but also the correct nonrelativistic wavefunctions (eigenvectors). Knowing the wavefunctions for both the initial and the final states the transition probabilities can be calculated by simply evaluating a certain matrix element between these functions

$$A_{if} \sim \langle \Psi_f | M | \Psi_i \rangle. \quad (2.19)$$

There are several different kinds of transitions that can take place and be evaluated [8]. The three most dominant ones are the electric dipole (E1), magnetic dipole (M1) and electric quadrupole transitions (E2). Whenever possible, depending on different angular selection rules, the E1 transitions is by far the most important type. The other ones may then be neglected. E1 transitions are therefore frequently called *allowed* transitions and the others *forbidden*. When the E1 transitions are forbidden, **then** weak M1 or E2 transitions may be important.

The matrix element between the wavefunctions for the initial and the final states, for E1 transitions, can be evaluated in at least [9] three different ways

$$\langle \Psi_f | \sum_i \mathbf{r}(i) | \Psi_i \rangle \quad (2.20a)$$

$$\frac{2}{E_i - E_f} \langle \Psi_f | \sum_i \nabla_i | \Psi_i \rangle \quad (2.20b)$$

$$\frac{2}{(E_i - E_f)^2} \langle \Psi_f | \sum_i \nabla V_i | \Psi_i \rangle \quad (2.20c)$$

These forms are called the *length*, *velocity* and *acceleration* forms, respectively. For exact total wavefunctions these matrix elements are equivalent, but when approximate wavefunctions are used they usually give rather different results. The acceleration form is normally the most unreliable one, and is very sensitive to the form of the wavefunction close to the nucleus. This form is not used at all in the work presented in this thesis.

The simplest one to use in practical computations, and the most commonly used, is the length form. In this form the integrand is weighted towards large r values, which can be particularly suitable when using certain atomic models. This will be discussed later.

Radiative lifetimes for a number of atomic states are measured and reported on in this thesis: for Ga in papers IV, V and IX and for Sr in papers VII and VIII. The *ab initio* calculations for transition probabilities in Ga, (papers IX and X) are evaluated using the length form of the dipole operator. The velocity form was also used but only to check the approximate wavefunctions. Obtaining similar results with the two forms does not guarantee accurate wavefunctions [10] but if the differences are large some important effects must surely have been omitted when constructing the approximate wavefunctions.

3 EXPERIMENTAL TECHNIQUES

The atomic structures and radiative properties, upon which the work presented in this thesis is based, have been studied experimentally using several quite different methods. For the analysis of the gross and fine energy structures of Sr, Rb and Xe ions (papers I,II and III) several hundreds of spectral lines were recorded to give enough material for the determination and classification of the large number of different energy levels.

In the hyperfine structure measurements (papers IV to VII), on the other hand, the substructure of sometimes only one of the fine-structure levels, is subject to investigation. The requirements placed on the experimental set-up are then quite different. The measurements require, not only higher resolution, but also some way of avoiding the Doppler broadening of the spectral lines.

Still different methods are used when radiative properties, such as lifetimes, are to be investigated (papers VII to IX). The method chosen then often depends on whether relative transition probabilities are sufficient or if absolute values are required. The desired accuracy is another crucial factor when selecting the experimental method.

3.1 ENERGY LEVEL SYSTEM

To obtain the emission spectra of atoms or ions a light source [11] of some kind is needed, within which the atoms are excited, or ionized if ionized states are to be studied. The spectra can then be recorded by using a spectrograph and photographic recordings.

LIGHT SOURCES

The choice of light source for a particular investigation is determined by many factors, such as the nature and availability of the material to be excited, the physical limitations, the intensity, lineshape and degree of excitation desired.

A commonly used source is an *electric arc* between solid electrodes. In the arc column, at some distance from the electrodes, predominantly lines emitted by the neutral atoms are obtained, (except for the more easily ionized atoms). In the region close to the electrodes the excitation is higher and lines of ionized atoms are often found.

The *spark* in many different modifications, is a source producing higher excitations and having greater flexibility. The spark, which is operating in vacuum, is produced by applying 10-50 kV across the electrodes which carries the test samples. The peak of the discharge current may easily be several thousand amperes. The result is an almost explosive emission of excited vaporized materials from the electrodes, and ionization stages as high as 8 - 15 are produced. When lower ionization stages (3 - 8) are to be investigated a *sliding spark* can be used. An insulator is then placed between the electrodes, shaped as a guiding tube for the spark between the electrodes. This will make the spark slide along the side of the insulator instead of in the empty electrode gap, and the break-through occurs at a much lower voltage across the electrodes. With the

spark, as well as the arc, any conducting solid electrodes may be used directly. Substances which are rare, nonconducting, powdered, in the form of salts or otherwise unsuitable for use as solid electrodes may be packed in a hollow, conducting electrode, alloyed with other materials, or pressed or sintered with metal powders into solid electrodes.

By keeping a gas at low pressure between and around the electrodes a steady gaseous discharge can be obtained. This is used in the *hollow-cathode discharge tube*. The cathode may be made of the material to be excited, if it is a material with suitable physical properties. Other materials may be placed inside a hollow cathode made of a suitable material. The low pressure and low electric fields used, and the possibility of cooling, make the hollow cathode one of the best light sources for emission spectroscopy when high resolution is needed. A drawback of the hollow-cathode is that it is difficult to classify the spectral lines according to ionization stages.

By placing a closed vessel inside a coil carrying a high-frequency current, a gaseous discharge may also be maintained without any electrodes. This is especially convenient in investigations of rare gases or gases and vapours which attack the electrodes or which may be contaminated by them.

The discharge tube in a *theta pinch discharge* [12] is surrounded by a coil carrying pulses of very high current ($\sim 100\,000$ amperes). The plasma is compressed by the high magnetic field produced by the coil, and relatively high ionization stages can be produced. The degree of ionization can conveniently be varied, and this makes the theta pinch very valuable in the classification of spectral lines with respect to ionization stage.

A completely different type of "light source" is used in *beam-foil spectroscopy* [13]. There ions are accelerated in a particle accelerator to high velocities ($\sim 10^6$ m/s), and sent through a thin foil of e.g. carbon where electrons are either picked up, or stripped off. This method is well suited for the production of ions of high ionization stages. The ions (or neutral atoms) are left in different excited states and will, on their continued path behind the foil, emit the light which is to be analyzed.

For the work on emission spectroscopy presented in this thesis, (papers I, II and III) several different light sources were used. The Sr V and Rb IV spectra were produced in a sliding spark whereas a theta-pinch discharge, DC hollow cathode and a Xe laser tube without end-mirrors were used for the production of the Xe III spectra. For extra reference spectra, light from additional hollow-cathode discharges were superimposed.

SPECTROGRAPHS

Many different ways of arranging, - mounting - , the entrance slit, grating, focusing system and photographic plate in spectrographs exist; each having their own advantages and drawbacks [14]. The choice of mounting depends primarily on the wavelength range of the spectra to be investigated, and the desired resolution. In, for example, the recording of the Rb IV spectra, reported on in this thesis, three different spectrographs were used to cover the spectral range of interest.

There are different mountings for plane and concave gratings. In the short wavelength part of the ultraviolet region grazing incidence arrangements are used to increase the reflectivity of the grating. Plane gratings are used in e.g. the Ebert spectrograph where mirrors are used as a focusing device. For wavelengths shorter than ~ 200 nm light is absorbed by air, and the spectrograph must be evacuated.

3.2 HYPERFINE STRUCTURE

Hyperfine structure investigations require higher resolution than the spectral recordings described above. Due to the width of the spectral lines, the use of a spectrograph with higher resolving power is not always sufficient.

LINE BROADENING

The finite width of the spectral lines is due to a number of factors [15]. For excited states, having a finite lifetime, the Heisenberg uncertainty relation gives a finite uncertainty in the energy of the excited state. This results in a natural halfwidth of the spectral lines inversely proportional to the radiative lifetime. For example, the gallium resonance line connecting the ground state and the $4d\ ^2D$ state with $\tau \approx 7$ ns (paper IX and X) has a natural linewidth of ~ 20 MHz. The spectral line from the forbidden $2s\ ^2S$ to $1s\ ^2S$ transition in hydrogen, on the other hand, has a natural linewidth of only $\delta\nu = 0.15$ Hz. This is due to the very long lifetime of the metastable $2s\ ^2S$ state ($\tau \sim 1$ s).

Generally, the most serious broadening mechanism, when not reduced by some means, is *Doppler broadening* due to the random motion of the atoms relative to the observer. The Doppler broadening of spectral lines from thermal light sources is often of the same size or even greater than the hyperfine structures, and special techniques are therefore often required for hyperfine structure investigations.

Another contribution to the spectral linewidth is *pressure broadening*, if collisions between the atoms in the source are frequent. *Stark broadening* occurs if high electric fields are present, as in arcs or sparks, or if there are frequent collisions with ions. (Atoms excited to high Rydberg states may also be very sensitive to weak electric fields [16]). In laser experiments the interacting radiation field may be very strong causing *saturation broadening*. If the radiation field interacts with the atoms for a time shorter than the natural radiative lifetime, so-called *time-of-flight-broadening* may occur.

RF RESONANCE METHODS

There are a number of different methods developed for high-resolution spectroscopy [17]. Several different resonance methods, such as atomic beam magnetic resonance (ABMR), for ground and metastable states, and optical-radio-frequency double resonance for excited states, are well suited for high-resolution investigations of e.g. hyperfine structures. With these methods the hyperfine energy splittings are not determined by comparing the wavelengths of the optical transitions to (or from) the different levels involved. Instead the

frequency of a radiation field inducing transitions between the different hyperfine levels is measured. The Doppler width of a spectral line is proportional to the frequency of the transition. If the RF transitions of frequency ν_{RF} ($\nu \sim 10^9$ Hz) are studied instead of the optical ones, having much higher frequency ν_{opt} ($\nu \sim 10^{15}$ Hz), the broadening is reduced by a factor $\nu_{\text{opt}}/\nu_{\text{RF}}$. The Doppler broadening is not totally removed, but reduced to an extent where it can usually be neglected compared with the other broadening mechanisms.

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There are several experimental schemes for high-resolution, sub-Doppler, spectroscopy [18] which are based on the special characteristics of tunable single-mode dye lasers [19]. The large spectral power density, the possibility of continuously tuning the wavelength and the extremely narrow spectral linewidth make these lasers excellent tools for high-resolution investigations. The spectral resolution available with single-mode dye lasers may exceed that of the largest spectrographs by several orders of magnitude.

COLLIMATED ATOMIC BEAMS

One way of performing sub-Doppler spectroscopy on, e.g. hyperfine structures, is to use a collimated atomic beam. Here a beam of free atoms is produced, for example, by vaporization in an oven, of the element to be investigated. The evaporated material then effuses into a vacuum chamber through a small hole. By varying the temperature in the oven, the atomic density can easily be controlled. The beam is further collimated by one or several apertures. The atoms in the beam are excited by light from the dye laser, and the entire hyperfine structure is covered in a continuous sweep of the laser wavelength. (Sometimes two lasers are needed for step-wise excitation.) When the laser light is in resonance with a transition to one of the hyperfine components excitation occurs, and this is observed by monitoring the light emitted in the spontaneous decay following the excitation.

By exciting at right-angles to the direction of motion, the Doppler effect is substantially reduced. In all practical cases, a compromise must be made between strong collimation and signal strength. Reducing the first-order Doppler broadening completely would, in principle, require an infinitely narrow atomic beam and hence practically no atoms would be left to interact with the laser beam.

Simultaneously with the fluorescence light from the atoms, the signal from an interferometer with well known free spectral range is recorded as a reference for the evaluation of the recorded spectra. The absolute value of the energies of the levels are not obtained, nor the exact wavelengths of the exciting or detected light, but the hyperfine *splittings* are.

The method described above was used for the hyperfine structure measurements on excited ^2P states in Ga and on some perturbed ^2D states in Al, Ga and In, reported on in this thesis in papers IV and VI.

DOPPLER-FREE SATURATION AND POLARIZATION SPECTROSCOPY

Two other types of techniques for Doppler-free laser spectroscopy which should be mentioned briefly here are *Doppler-free saturation* and *polarization spectroscopy*. The atoms to be investigated with these methods may be kept inside a hollow cathode or a cell with low gas pressure. By using two counter-propagating laser beams, with the same frequency, a pump beam and a probe beam, Doppler-free signals can be obtained.

The frequency ν of the light in the laser beams is tuned close to resonance, ν_0 , for the transition to be investigated. Only atoms in velocity groups where the detuning from resonance is compensated for by the Doppler shift, will experience a resonant radiation field. The only possibility for atoms in the same velocity group to interact with both beams is when their Doppler shifts are zero (or smaller than the natural width of the transition) *and* the laser frequency is tuned to resonance ν_0 . If the pump beam, in some way, marks the atoms it interacts with, Doppler-free signals can be obtained if the interactions, or absence of interactions, between atoms in the marked group and the counter-propagating probe beam are monitored.

In Doppler-free saturation spectroscopy the method of "marking" a velocity group by the pump beam is through "hole burning" in the velocity distribution. The number of atoms in the lower state, with a specific velocity in the direction of the pump beam, is decreased through excitation by the laser light. The counter-propagating probe beam is therefore less attenuated along the path through the cell if it interacts with the same velocity group as the pump beam. By monitoring the intensity of the probe beam after passing the cell, as a function of the laser frequency, a Doppler-free peak in intensity will occur at the transition frequency. In practice several modifications to the basic arrangement described above are used to increase the sensitivity [20].

In polarization spectroscopy, on the other hand, polarized light is used in the pump as well as in the probe beam. The pump beam will here (besides a certain hole-burning) induce an orientation, or alignment of the angular momenta of the atoms it interacts with and thereby mark a specific velocity group. If the counter-propagating, linearly polarized probe-beam interacts with the same velocity group as the pump-beam, then these oriented or aligned atoms will change the state of polarization. A Doppler-free signal is therefore obtained if the probe-beam is observed after passing an analyzer, oriented perpendicular to the initial plane of polarization. (In practice there will always be a certain background signal as crossed polarizers only have a finite extinction and because the state of polarization will also change due to small birefringence in the cell windows.) Polarization spectroscopy can also be modified in several ways and the sensitivity increased by e.g. modulation and lock-in techniques [21].

QUANTUM BEAT SPECTROSCOPY

The above described methods, as well as e.g. Doppler-free multiphoton spectroscopy [22], are based on the narrow spectral linewidth of tunable single-mode lasers. Another, quite different method for measurements of small energy substructures, such as hyperfine structures, is the *quantum beat technique* [23].

This method is based on the time evolution of the wavefunction of a coherently excited superposition of eigenstates with slightly different energies. All (or at least two) of the substates in the upper state to be investigated are excited coherently by e.g. a short laser pulse. The spectral width of the pulse must be large enough to coherently excite the different substates, so the laser light must not be monochromatic in this technique. (Coherent excitation can also be obtained by other methods such as beam-foil excitation.) The time evolution of the excited state, being a superposition of the energetically different substates will give intensity modulations, *quantum beats*, in the fluorescence decay light. The frequencies of these quantum beats are proportional to the energy splittings between the different substates.

If the beat frequencies are measured, this method allows determination of the energy separation of the levels even if the separation is less than the Doppler width in the optical transitions. This requires a fast time-resolved detection system such as a photomultiplier tube and a box-car integrator or transient digitizer. When more than two energy levels are present, a Fourier transform of the time-resolved fluorescence intensity gives the frequencies corresponding to the different energy separations.

The quantum beat method is not strictly Doppler-free. But in the same manner as for the RF-resonance methods mentioned above, the observed frequencies are not in the optical region but rather in the RF-region resulting in correspondingly much narrower Doppler profiles.

There are experimental limitations both on the excitation and the detection side for the size of the energy splittings which can be investigated with the quantum beat method. The separations between the levels must not be larger than the spectral width of the exciting light as the eigenstates must be coherently excited. Short duration of the laser pulses (typically 1-10 ns) causes the fundamental Fourier broadening of the radiation to be in the range 0.1-1 GHz. In practice the limitations are therefore usually on the detection side. The energy splittings must be small enough so that the resulting beat frequencies do not become so large so that they can not be resolved and recorded by the detection system. When the quantum beats are recorded by a photomultiplier tube and a transient digitizer or box-car integrator, the upper limit should be somewhere around 200 MHz. (The detection system used in the quantum beat measurements reported on in this thesis has an upper limit of approximately 50 MHz.)

Whenever this method is applicable, bearing in mind the limitations mentioned above, it is a very powerful technique. As a narrow bandwidth is not required, pulsed lasers with high pulse power may be used, and several means of short wavelength generation become available. The high pulse power facilitates e.g. frequency doubling, tripling, mixing, and Raman shifting of the laser light [24].

However, there is one drawback with this technique (and with, e.g., the *level-crossing* technique [25],); only the *absolute values* of the energy separations can be determined. When measuring hyperfine structures, the signs of the deduced hyperfine coupling constants, A and B, will be undetermined. Here accurate absolute values from the measurements can be combined with signs obtained from *ab initio* theoretical calculations.

Quantum beat spectroscopy was employed for the hyperfine structure measurements in the $np\ ^2P$ sequence in neutral Ga presented in this thesis (paper V).

3.3 RADIATIVE LIFETIMES

There are a number of different methods [26] for experimental investigations of radiative properties. In an energy structure investigation using spectrographs and photographic recordings some indications of the strengths of the individual transitions are obtained by the degree of blackening on the photographic plates. Relative oscillator strengths are often determined in this way. The accuracy is rather limited, however, since the blackening depends on several factors besides the intrinsic radiative properties of the atom. One important factor is the spectral sensitivity of the photographic plates. Another factor is the population of the different excited states. The population distribution among the excited states of atoms excited in e.g. a spark is not very well known and unambiguous interpretations of the blackening of the spectral lines become impossible. The evaluation of lifetimes usually requires the knowledge of a large number of oscillator strengths, and often for transitions in quite different wavelength regions. Accurate determination of radiative lifetimes for excited states by this method is therefore not at all possible.

BEAM-FOIL EXCITATION AND TRANSIENT RECORDING

Another, more direct method for lifetime determinations is the "beam-foil method", which was described briefly in the section on light sources. Instead of investigating the spectrum of the light emitted directly after the excitation in the foil, the intensity of the light from one particular transition is recorded as a function of the distance from the foil along the beam. If the velocity of the atoms, or ions, in the beam is known, the intensity as a function of time after excitation can easily be deduced. By fitting an exponential function and a background to the recorded intensity curve, the radiative lifetime of the upper level can be determined. A complicating factor with this method is the simultaneous decay of higher states causing cascade population of the level to be investigated. The intensity of the light, as a function of time, is therefore often a sum of several exponentials.

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There are also a number of methods based on e.g. the Hanle effect [27], where the width of the resonance signals is inversely proportional to the radiative lifetimes of the energy levels. By measuring the width, the lifetime can be deduced.

Using lasers for excitation makes several very accurate techniques for lifetime measurements available. The narrow bandwidth of lasers permits the selective excitation of one particular state of interest at a time. The problem of cascades from higher levels is therefore avoided.

SELECTIVE EXCITATION AND TRANSIENT RECORDING

An experimental set-up similar to the one described above for quantum beat spectroscopy can be used. The atoms are selectively excited to a particular state by a short laser pulse. After the excitation light has been turned off, the fluorescence light is detected by a fast detector and recorded by e.g. a box-car integrator or a transient digitizer. To obtain good signal-to-noise ratios, the signals from a large number of decays are usually summed before evaluation. The lifetime is obtained by fitting an exponential function and a background to the obtained decay curve.

When using this technique it is important to take into account the earth's magnetic field which may induce small Zeeman splittings. These in turn give rise to Zeeman quantum beats of low frequency which may lead to erroneous lifetime evaluation when fitting the exponential.

In wavelength regions where only very low laser power is available, it is tempting to increase the density of atoms in the atomic beam (or cell) to obtain a reasonable signal-to-noise ratio. However, the excited state may then be depopulated by collisions with other atoms in the beam and the recorded decay curve will indicate a "lifetime" shorter than the true spontaneous lifetime. If the state to be investigated is connected by an "allowed" transition to the ground state, or a lower metastable state, another possible error source is *multiple scattering*. A photon emitted some time after the laser excitation might be re-absorbed by atoms in the lower state, and emitted at a later time. In this way an increased number of photons reach the detector at the later part of the decay curve, and the recorded "lifetime" will be longer than the true spontaneous lifetime. To eliminate these sources of error the atomic density must be kept sufficiently low.

If the measurement is performed at room temperature, there will be a background field due to black-body radiation present in the measuring volume. When comparing experimental and theoretical lifetimes of high-lying Rydberg states, it is therefore important to estimate the size of this effect which has the effect of shortening the recorded lifetime. In paper IX, *black-body-induced transitions* are discussed for the Ga states investigated.

If pulsed lasers are used, high pulse power and short wavelengths can be generated, as mentioned above, making this technique very useful. The lifetimes reported on in paper V, and some of those in papers VIII and IX, were obtained in the way described above. The method is, however, sensitive to e.g. nonlinearities in the detector, a problem which is eliminated if a delayed-coincidence method is used.

DELAYED COINCIDENCE

The lifetimes reported on in paper IV, and some of those in papers VIII and IX, were obtained using a delayed coincidence method, called *Pulse Modulated Laser Spectroscopy*, PUMOLS [28], which is outlined below. Also in this technique the laser pulses excite free atoms in a low-pressure cell or atomic beam. The excitation pulse starts a voltage ramp in a Time-to-Amplitude Converter, TAC, which is stopped by the first fluorescence photon detected after the excitation

pulse. The voltage pulse from the TAC is therefore proportional to the time between the excitation pulse and the detection of the fluorescence photon. This TAC-pulse is stored in a multichannel analyser, MCA, where each channel represents a certain voltage. By making the probability for detecting a photon per excitation pulse small compared with one, the probability of two photons arriving at the detector during one cycle is negligible. (A second photon would not be detected and erroneous results could be obtained.) After a large number of excitation pulses the voltage distribution on the MCA displays the decay curve directly.

Since, on average, less than one fluorescence photon per excitation pulse is recorded in this technique, a very large number of pulses are required for one decay curve with an acceptable signal-to-noise ratio. To make the measuring time reasonably short, high pulse frequencies are therefore desired. The repetition rates of pulsed lasers are usually much too low (typically 10 Hz). Instead the light from continuous lasers is pulse-modulated by a fast chopper or an acousto-optical modulator. Alternatively, a mode-locked laser may be used (paper IX) giving high repetition rates (typically 50 - 100 MHz) and very short pulses (less than 0.1 ns).

4 THEORETICAL METHODS

As already mentioned, there is no way of solving the Schrödinger equation (2.1) directly for a many-electron atom using the full Hamiltonian. A problem often encountered in theoretical atomic physics is therefore to make appropriate approximations and simplifications to the total Hamiltonian. The atomic interactions of interest must be reasonably well represented for the solution to be of any value. The Hamiltonian must, at the same time, be simple enough for the problem to be solvable. Another task for the theoretical physicist is to develop and improve computational methods for the numerical evaluation of approximate energy eigenvalues and eigenfunctions (wavefunctions). The theoretical method, or approach, best suited for a particular problem depends on the number of eigenstates and eigenvalues to be determined, the physical interactions of interest and on the accuracy required.

In an investigation of the gross energy level structure, the energies of hundreds of levels might be of interest, while e.g. the hyperfine structure of the individual fine structure levels is neglected. This requires a computational method, such as energy-matrix diagonalizations, that in an effective way gives the whole energy spectrum of interest. In other cases, the hyperfine structure of only one or a few fine structure levels might be the purpose of the entire investigation. Higher accuracy is then required, but normally only for the relative position of the different hfs levels. Computational methods based on perturbation theory to higher orders, variational techniques, or a combination of these, can then be used.

In some cases the energy structures are well known from experimental investigations. The purpose of solving the Schrödinger equation can then be to test atomic theories and computational methods, or to obtain the wavefunctions. These can then be used to obtain theoretical designations of the energy levels, or for calculations of atomic properties such as radiative transition probabilities or Landé g_J -factors. In such cases the *ab initio* wavefunctions can be optimized by varying the functions, or the parameters on which they depend, to minimize the differences between the experimental and theoretical energy eigenvalues.

The theoretical work presented in this thesis makes use of a number of quite different methods. It is, however, outside the scope of this presentation to give any detailed description of these different methods. The main goal of this chapter is rather to present the methods used, and briefly a few others, and to relate them to each other, and in this way motivate the choice of method for each of the different investigations.

A common feature of the different methods used is the need for reasonably good basis functions. The better the basis functions resemble the true wavefunction, the smaller the effort required to reach a certain accuracy. In most of the theoretical work presented in this thesis (*restricted*) *Hartree-Fock* (HF) basis functions were used and they will therefore be given some special attention.

HF functions are obtained by solving the *Hartree-Fock equations* by *self-consistent field* (SCF) methods. The Hartree-Fock equations are in turn obtained

by combining the *central-field model* (CFM) and the *variational principle*. These concepts are also quite important for the understanding of other parts of the work presented in this thesis, and will therefore be described briefly in this presentation.

4.1 THE CENTRAL-FIELD MODEL

The central-field model of the N-electron atom, is a special type of *independent particle model* (IPM). In IPM's the approximation made is that any given electron, i , moves independently of the others in the electrostatic field of the nucleus (assumed to be stationary) and the other N-1 electrons. The "best" IPM is the unrestricted Hartree-Fock model (UHF). It is numerically a very complex method as the radial and angular (and spin) functions can not be separated. The complexity of models like UHF makes them impractical as starting points for accurate variational or perturbational calculations. Further simplifications to the model are required.

In the central-field model the electrostatic field is assumed to be time-averaged over the motion of the N-1 electrons, and therefore (neglecting correlation with the position of the i^{th}) to be spherically symmetric. This leads to considerable simplifications in the calculations.

The central-field model may be put on a mathematical footing by separating the Hamiltonian (2.2) in the following way

$$H = H_0 + V_{\text{es}} \quad (4.1)$$

The approximate Hamiltonian H_0 , being a sum of one-electron operators $h_0(i)$, represents an average interaction with the nucleus and the other electrons. The non-central part of the electrostatic interaction, V_{es} , causes departures from this single-particle description, and will be treated as a perturbation.

The main advantage of this separation is the mathematical simplifications which follow from spherical symmetry. The eigenfunctions of the one-electron operators $h_0(i)$ can be separated into radial, angular and spin functions.

$$\phi(r, \theta, \phi, m_s) = \frac{1}{r} P_{nl}(r) \cdot Y_{lm_l}(\theta, \phi) \cdot \sigma_{m_s}(s_z) \quad (4.2)$$

As a consequence of the spherical symmetry, this "*spin orbital*" is an eigenfunction of the one-electron angular momentum operators, $\mathbf{l}^2$, $\mathbf{s}^2$, $\mathbf{l}_z$ and s_z . Y_{lm} represents a wellknown spherical harmonic and σ_{m_s} a two-valued spin function [29]. The "only" unknown is the radial function $P_{nl}(r)$.

The most straight-forward method of forming an N-electron wavefunction for the whole atom is to take a simple product of N different spin orbitals. However, these simple product functions do not fulfil the requirement that the wavefunction be antisymmetric upon interchanging the coordinates of any two electrons. Antisymmetric wavefunctions can be formed, however, by making certain linear combinations of product functions with all possible permutations of the coordinates. Such linear combinations can be written in the form of a determinant [30], and is referred to as a *determinantal function* or a *Slater determinant*. Antisymmetrization, the Pauli principle and certain correlation

effects (between electrons with parallel spin) then follow directly from the well-known properties of determinants.

If one (or several) shells are open, there are normally many determinants belonging to the same configuration. The energy eigenvalue of a single electron in a central-field depends only on n and ℓ . In the central-field approximation therefore, all states belonging to the same configuration are degenerate. The non-central part of the Coulomb interaction V_{es} is diagonal with respect to the total orbital and spin angular momenta, L and S . When calculating the effect of V_{es} using first-order perturbation theory different energies are obtained for the different LS terms. Eigenfunctions with definite angular momentum symmetry are formed as linear combinations of determinants belonging to the same configuration but with different magnetic quantum numbers m_ℓ, m_s . (This is the well-known LS or *Russel-Saunders* coupling).

The evaluation of the radial integrals for the Coulomb matrix element in the perturbation calculation is straightforward and unaffected by angular momentum coupling. The evaluation of the angular part, on the other hand, can, in the general case, be quite cumbersome and difficult. Racah algebra ("Racah-Wigner algebra" or "the algebra of irreducible tensor operators") [31] provides notational and calculational simplifications of great elegance, which are practically indispensable for the evaluation of matrix elements for complex configurations. It would however be outside the scope of this short presentation to describe this technique.

General expressions for the first-order energy of a particular LS term $E(LS)$ or for the average over all the terms within the configuration E_{ave} can be derived [32]. These may be expressed in terms of angular coefficients, obtained using Racah algebra, and one-electron radial integrals, $I(n\ell)$ and two-electron radial Slater integrals, $F^k(n_i\ell_i, n_j\ell_j)$ and $G^k(n_i\ell_i, n_j\ell_j)$ given by (using the abbreviation ij for $n_i\ell_i, n_j\ell_j$)

$$I(n\ell) = \int_0^\infty P_{n\ell}(r) \left[-\frac{1}{2} \frac{d^2}{dr^2} + \frac{\ell(\ell+1)}{2r^2} - \frac{Z}{r} \right] P_{n\ell}(r) dr \quad (4.3a)$$

$$F^k(i, j) = R^k(ij, ij) \quad (4.3b)$$

$$G^k(i, j) = R^k(ij, ji) \quad (4.3c)$$

$$R^k(ab, cd) = \int_0^\infty \int_0^\infty P_a(r_1) P_b(r_2) \frac{r_1^k}{r_2^{k+1}} P_c(r_1) P_d(r_2) dr_1 dr_2 \quad (4.3d)$$

In spectroscopic work the main interest often lies not in the absolute energy of the levels, but rather in their relative positions. It is therefore convenient to express the LS term energies relative to the configuration average as

$$E(LS) = E_{ave} + \Delta E(LS) \quad (4.4)$$

This simplifies the computational work considerably since the expression for $\Delta E(LS)$ only involves the two-electron Slater integrals and only for electrons in open subshells.

The spin-orbit interaction, which is diagonal with respect to the total angular momentum j_i , can similarly be treated as a perturbation. In many cases, especially for neutral atoms with low Z , it is sufficient to treat this effect as a "weak" interaction compared with the non-central Coulomb interaction. The individual LS terms are then split into different fine structure states. Each of these has a certain total angular momentum J , and a certain total energy, $E(\text{LSJ})$.

In other cases the spin-orbit interactions are comparable to the non-central part of the Coulomb interaction. States with the same J value but with different L and S are then mixed to a large extent. In such cases the technique of energy-matrix diagonalization (section 4.4) is well suited for the calculation of energy eigenvalues and eigenvectors.

In atoms with very high Z , the spin-orbit interaction may dominate over the non-central Coulomb interaction. $\mathbf{l}_i$ and $\mathbf{s}_i$ are then coupled to a total angular momentum, j_i , for each electron, and these then couple to form a total J for the atom (*jj coupling*).

The LS coupling notation has been utilized in all the papers presented in this thesis. In the three investigations of ion spectra, however, (papers I, II and III) many of the terms investigated were found to be strongly mixed. When calculating radiative lifetimes for some excited states in neutral Ga, on the other hand, (papers IX and X) the effects of the spin-orbit interactions were neglected when computing the wavefunctions. (The dominant configuration in each calculation had only one electron outside closed shells, and therefore only one (*pure*) LS term.)

As is evident from the discussion above, a great deal of atomic structure can be calculated if the radial one-electron functions $P_{nl}(r)$ are known. To obtain the Hartree-Fock equations for the radial functions, the central-field energy expression for E_{ave} (or $E(\text{LS})$), outlined above, is combined with the variation principle to be discussed next.

4.2 THE VARIATIONAL PRINCIPLE

If any approximate wavefunction, (with proper functional form) is used to evaluate the expectation value of the Hamiltonian, it can easily be shown [33] that the value obtained will always be in excess of the true eigenvalue for the ground state. If the wavefunction (or parameters on which it depends) is varied until the expectation value of the energy reaches a minimum, then the "best" approximate ground-state wavefunction is obtained (within the limitations set by the functional form used). This is *the variational principle* on which several variational methods are based.

If an excited state, for which the wavefunction is to be calculated, can be characterized as being the lowest state of e.g a certain parity or angular momentum, then the principle can also be applied directly to such states. Variational methods can, however, be used in more general cases. Use is then made of the *Ritz theorem* [34] which states that *the expectation value of the Hamiltonian H is stationary in the neighborhood of its discrete eigenvalues.*

4.3 THE HARTREE-FOCK METHOD

As outlined above, the energy for a given configuration (E_{ave}) or LS term ($E(\text{LS})$), can, within the central-field model, be given in terms of integrals of the one-electron radial functions in the spin orbitals. The Hartree-Fock radial functions are defined such that the expectation value of the energy is stationary

$$\delta \langle E \rangle = 0 \quad (4.5)$$

for small changes in *any* of the *radial* one-electron functions. The orbitals should be orthonormal and satisfy certain boundary conditions at the origin and infinity, and this places some restrictions on the possible variations. These restrictions on δP_i can be relaxed considerably, with normalization and orthogonality still preserved, by including suitable Lagrange multipliers [35] ϵ_i and λ_{ij} in the stationary expression

$$\delta \left[E - \sum_i (q_i \epsilon_i \int_0^\infty P_{n_i l_i}(r)^2 dr) - \sum_{i \neq j} q_i q_j \lambda_{ij} \delta(l_i l_j) \int_0^\infty P_{n_i l_i}(r) P_{n_j l_j}(r) dr \right]. \quad (4.6)$$

Here q_i equals the number of electrons in the i^{th} subshell, and the summations are performed over all the subshells and not over the individual electrons. (This is one of the simplifications which follows from the central-field approximation.) $\delta(l_i l_j)$ is a Cronecker deltafunction with respect to the orbital quantum numbers.

The Hartree-Fock equations are obtained from (4.6) by considering the variations in the radial integrals $I(i)$, $F^k(i,j)$ and $G^k(i,j)$, present in the expression for the energy, with respect to any small variation δP_i , of the function P_i .

The Hartree-Fock equations obtained can be written [36] (leaving out the off-diagonal Lagrange multipliers, λ_{ij})

$$\left[-\frac{1}{2} \frac{d^2}{dr^2} + \frac{l_i(l_i + 1)}{2r^2} - \frac{Z}{r} + U_{\text{HF}}(r) \right] P_i(r) = \epsilon_i P_i(r).$$

The Hartree-Fock potential U_{HF} used here is defined by

$$U_{\text{HF}}(r) P_i(r) = \sum_j q_j \left[c(ijk) \frac{1}{r} Y_k(jj,r) \cdot P_i(r) + d(ijk) \frac{1}{r} Y_k(ij,k) \cdot P_j(r) \right] \quad (4.7)$$

where

$$Y_k(ij,r) = r \int_0^\infty \frac{r_{<}^k}{r_{>^{k+1}}} P_i(r') P_j(r') dr' \quad (4.8)$$

and $r_{<}$ is the smaller and $r_{>}$ the greater of the two radial distances r and r' .

The first part of eq. (4.7) represents the direct interaction, and the second the non-local exchange interaction. The effect of this potential on an orbital at a certain radius also depends on the orbitals at other radii, via the Y_k functions. This *nonlocality* is numerically a complicating factor in the HF equations.

Since the i^{th} HF equation involves P_j for all j , we have a set of Q (Q =number of occupied subshells) coupled integro-differential equations that (if $Q > 1$) can be solved only by an iterative procedure. Each iterative cycle consists of

- * assuming a set of trial functions $P_j(r)$, $1 \leq j \leq Q$
- * computing the Y_k (and estimating ϵ_{ij}) for each i
- * numerically solving the i^{th} HF equation for a new, normalized $P_i(r)$, for each i .

These three steps are repeated, using an improved set of trial functions each time, until the output functions obtained in the last step are identical to the functions assumed in the first within the desired tolerance. The output functions are then self-consistent with the trial input functions, and the procedure is called a *self-consistent-field* (SCF) method.

The solution of the inhomogeneous Hartree-Fock equations is numerically quite complex, and complications and instabilities can occur. However, having access to fast computers and the excellent computer codes by e.g. C. Froese Fischer [37], the calculation of the (single-configuration) HF radial functions needed for the work presented in this thesis, e.g. in papers I-III, V and VI, caused very few difficulties. With only a few exceptions, this part of the work was quite straightforward.

There exist many different local approximations of U_{HF} , [38] each with different advantages and drawbacks. They all avoid the inhomogeneous equation through different approximations of the exchange interaction. The numerical procedures are therefore simplified and speeded up considerably. Examples of such *local potential approximations* are the *Hartree* (H), *Hartree-Fock-Slater* (HFS) and the *Hartree-Slater* (HS) methods.

When calculating correlation effects using many-body perturbation theory (paper V) nonlocal Hartree-Fock as well as local Hartree-Fock-Slater potentials were used.

It is not only term- and fine structure splittings that can be evaluated with first-order perturbation theory from the HF (CFM) wavefunctions. Using the hyperfine operators (2.11) and (2.12) a first-order estimate of the atomic hyperfine interaction can be evaluated. As a consequence of the spherical symmetry of the closed shells, the summation need only be performed over electrons in open shells. In Ga (paper V), for example, the experimental A factor for the $4p^2 P_{3/2}$ state (191 MHz) was found to be relatively well represented by the HF value of 195 MHz. For the $J=1/2$ state, on the other hand, the deviation is considerably larger. Exceptionally large deviations are reported in paper VI. The

HF value for $A(^2D_{3/2})$ for the $3s^2 3d^2 D_{3/2}$ state in Al, for instance, is +1.0 MHz, whereas the value observed was -99 MHz.

Using the dipole operator (2.20) (usually the length form (2.20a), is preferred) and single-configuration HF wavefunctions, first-order transition probabilities can be calculated. It was found (papers IX and X) that the radiative transition probability between the lowest term in neutral Ga, $4s^2 4p^2 P$ and the excited $4s^2 8d^2 D$ term is strongly suppressed as a result of the correlated motion of the electrons in the 2D state. Using the single-configuration HF model for the 2D state would give a transition probability about 200 times larger than the value obtained in a more accurate calculation. On the other hand, the HF value for the transition probability between the lowest term and the $4s^2 8s^2 S$ term represents the "exact" value within 20%.

The term- and fine structure splittings are also sensitive to higher order effects. In papers I, II and III a large number of examples can be found that demonstrate the need to include effects beyond the single-configuration model to describe these splittings properly.

As is evident from the discussion above, reliable calculations often require sophisticated methods, taking into account the correlated motion of the electrons and polarization of the closed core. (Some authors define *correlation* to be the entire difference between HF and experiment). However, in most cases the single-configuration HF model represents the physical reality well enough to be a suitable starting point for an accurate perturbation calculation (section 4.7), and the wavefunctions can be used as basis functions when configuration interactions are taken into account in e.g. an energy-matrix diagonalization (section 4.4 and 4.6).

4.4 ENERGY MATRIX DIAGONALIZATION AND PARAMETRIC FITS TO ENERGY LEVELS

For gross and fine structure calculations we want to solve the Schrödinger equation for a large number of states. Most commonly some variation of Slater-Condon theory is used [39]. The basic procedure consists of expanding the unknown wavefunction, Ψ^k , in terms of a set of known basis functions, ϕ_i , which may belong to different configurations (with the same parity),

$$\Psi^k = \sum_i c_i^k \phi_i. \quad (4.9)$$

The basis functions are assumed to be members of a complete set of orthonormal functions;

$$\langle \phi_i | \phi_j \rangle = \delta_{ij}. \quad (4.10)$$

In general, this set has an infinite number of members, and so in principle (4.9) represents an infinite series. In practice, it is necessary to truncate this series to a finite number (M) of terms. It is then essential that the basis functions be of an appropriate type, and that the particular functions to be included in (4.9) in any given case be chosen judiciously.

Let $\mathbf{H}$ denote the matrix with the matrix elements

$$H_{ij} = \langle \phi_i | \mathbf{H} | \phi_j \rangle \quad (4.11)$$

($\mathbf{H}$ is Hermitian and by choosing the basis functions to be real, $H_{ij} = H_{ji}$). The Schrödinger equation can then be transferred to the matrix equation

$$\mathbf{H} \mathbf{C}^k = E^k \mathbf{C}^k \quad (4.12)$$

where $\mathbf{C}^k$ is a column vector giving the c_i coefficients in the truncated expansion (4.9) for Ψ^k .

$$\mathbf{C}^k = \begin{pmatrix} c_1^k \\ c_2^k \\ \vdots \\ c_M^k \end{pmatrix} \quad (4.13)$$

Once the Hamiltonian matrix elements have been computed, the problem of computing the eigenvalues and eigenvectors is essentially trivial. The difficulties lie in constructing an appropriate, finite, set of basis functions and evaluating the matrix elements of the Hamiltonian matrix. Using digital computers and standard numerical methods [40] the matrix $\mathbf{T}$, which diagonalizes the Hamiltonian matrix is found. The K^{th} diagonal element of the diagonalized energy matrix is the eigenvalue E^k , and the K^{th} column of $\mathbf{T}$ represents the corresponding eigenvector $\mathbf{C}^k$. In practice the total matrix is divided into a number of submatrices, one for each value of J (or F) since states with different total angular momentum can not interact.

This technique was used when investigating the energy level structure of Sr^{*+} , Rb^{3+} and Xe^{2+} (papers I, II and III). The Hamiltonian included the non-central electrostatic Coulomb interactions as well as the spin-orbit interaction. As basis functions LS-coupled single-configuration functions were used, and the radial parts were obtained by the HF method for E_{ave} . Racah algebra and radial Slater integrals were used to evaluate the Hamiltonian matrix elements [41].

In principle, there is no limitation on the accuracy obtainable with the above method. However, as the Hamiltonian matrix grows with the number of terms M in the truncated expansion (4.9), the limiting factor will eventually be the computer facilities available. When spin-orbit interactions can be neglected, one LS term can be treated at a time, and a considerably larger number of configurations can be included in the expansion (section 4.6).

When terms from several configurations are included in the expansion, the effect of *configuration interaction* (CI) can be investigated. Some of the important observations reported on in the above mentioned papers are related to some special properties concerning HF basis functions and configuration interaction. These properties are outlined in the next section where *Brillouin's theorem* is presented.

If the energy level structure, or at least parts of it, is known from experimental determinations, the *ab initio* wavefunctions can be improved by fitting the calculated energy levels to the observed by treating the radial integrals as free parameters. The initial "parameters" are adjusted, and the new energy matrix obtained is diagonalized. The differences between experimental and theoretical energies are compared again and the parameters readjusted and so on. This iterative process is continued until an optimum fit is obtained. The *least-squares parametric fitting method* described here was employed in the work discussed above (papers I, II and III) using a computer program originally designed by R.D. Cowan [42].

The fitted values obtained in this way are in some respect closer to "reality" than the HF values. For example, it was found in the analysis of $4p^3n\ell$ configurations in Sr^{++} and Rb^{3+} that the fitted value of the $F^2(4p,4p)$ integral, representing the Coulomb repulsion between two equivalent $4p$ electrons, was only about 80% of the HF value. This can easily be understood *qualitatively*.

Since the Hartree-Fock model is an independent particle model, each electron moves only in an average field of the other electrons. The motion of the "real" electrons, however, is correlated in their mutual Coulomb field. They try to avoid each other, and this has the effect of reducing their effective interaction.

There are certain difficulties with this method however. The initial estimate must be fairly good, or the task of "pairing" a certain experimental level to the correct eigenvalue of the energy matrix can be extremely difficult. In some cases, the deviation between the observed and calculated positions for close-lying levels might be such that the total fit, even in the final iteration, will be improved if the levels are incorrectly paired. The process of adjusting the parameters, and fitting the levels, must therefore be carefully guided by all the experimental information available concerning the levels.

4.5 BRILLOUIN'S THEOREM

Consider LS-coupled wave functions of two states belonging to two different configurations, c_1 and c_2 , in the same *Rydberg series*. This means that the configurations differ only in the n -quantum number of one electron, e.g. $4p^35d$ and $4p^36d$ in Sr^{++} (paper I). If $|c_1\gamma_1 \text{ LS}\rangle$ and $|c_2\gamma_2 \text{ LS}\rangle$ are orthogonal and satisfy

$$\langle c_1\gamma_1 \text{ LS} | H | c_2\gamma_2 \text{ LS} \rangle = 0 \quad (4.14)$$

they are said to obey Brillouin's theorem [43]. (Here H is the non-relativistic Hamiltonian including the kinetic energy and the electrostatic terms).

Basis functions usually obey this theorem if they are constructed from radial wavefunctions obtained by solving the Hartree-Fock equations for the LS term in question. This follows from the fact that the HF equations were derived from an energy variation principle. A simple "proof" of this property of HF-basis functions can be given as follows:

Suppose that $|c_1\gamma_1 \text{ LS}\rangle$ is the lowest-energy single-configuration state having a particular angular symmetry. Then, if the CI matrix element (4.14) were non-

zero, the resulting CI perturbation would produce an energy lower than the single-configuration value. However, since $|c_2\gamma_2 LS\rangle$ has the same angular form as $|c_1\gamma_1 LS\rangle$, then the mixed state can differ from $|c_1\gamma_1 LS\rangle$ only in its radial dependence. But the radial functions of $|c_1\gamma_1 LS\rangle$ are derived to be those giving the lowest possible energy, so this contradicts the assumption that the CI matrix element is non-zero.

It should be noted, however, that Brillouin's theorem as stated here only holds when the HF equations are derived for a given LS term. When using the HF equations for the configuration average, there can still be, as shown in papers I - III, important CI contributions for the individual LS terms.

4.6 CONFIGURATION INTERACTION METHODS

MULTI-CONFIGURATION HARTREE-FOCK

Here and in the next chapter different ways of calculating electron correlation will be treated. In the present chapter configuration interaction methods are outlined with emphasis on the multi-configuration Hartree-Fock method used in this thesis. In the next chapter the many-body perturbation approach is described briefly, with the applications to atomic hyperfine interactions emphasized.

The technique of expanding the wavefunction Ψ^k in terms of a set of known basis functions, ϕ_i ($i=1,2,\dots$), was outlined in section 4.4. In that section the emphasis was on investigations of gross energy level structures (e.g. papers I, II and III). The aims were to obtain, simultaneously, a large number of eigenvalues and to treat the spin-orbit interaction on equal footing with the non-central part of the Coulomb interaction. Some correlation effects were included by the inclusion of more than one configuration at a time in the expansion (4.9). The basic method, however, can also be used for more accurate calculations of wavefunctions including correlation effects.

The Hamiltonian used in the correlation methods described here includes only kinetic energy and electrostatic interactions. In this way, since the spin-orbit interaction is neglected, L and S are good quantum numbers, and the configuration interaction (CI) wavefunction takes the form

$$\Psi(LS) = \sum_{i=1}^M c_i \phi_i(\alpha_i LS) \quad (4.15)$$

where M is, in principle, infinite, but in all practical cases finite. α_i represents the coupling schemes of the "configurations". (In CI contexts, "configuration" represents not only the set of $n\ell$ quantum numbers, but also the coupling schemes). The configurations included in the expansion must all have the same parity.

The c_i coefficients may be determined by minimizing the expression $\langle \Psi | H | \Psi \rangle$ subject to the condition $\langle \Psi | \Psi \rangle = 1$. The condition for the energy to be an extremum, $\delta E = 0$, is the matrix eigenvalue equation

$$H C^k = E^k C^k. \quad (4.16)$$

This is a matrix equation of the same type as eq. (4.12) described in section 4.4, and the method of solving the equation is the same. In CI calculations non-orthogonal basis functions are frequently used, then an overlap matrix S , with $S_{ij} = \langle \phi_i | \phi_j \rangle$, can be included in the equation to yield

$$H C^k = E^k S C^k. \quad (4.17)$$

Any one of the energy eigenvalues can now be used as the functional to be minimized with respect to variations in the radial functions P_{nl} . There are, in principle, two different schemes used to perform this variation.

SUPERPOSITION-OF-CONFIGURATIONS

The *superposition-of-configurations* (SOC) method starts from the Hartree-Fock wavefunction for the configuration of interest. In this way a set of radial functions is defined which, without modification, is used in the formation of the remaining wavefunctions in the expansion. The formation of the remaining configurations, however, requires that this set of HF radial functions is extended with extra orbitals. The form of these extra orbitals is then optimized to minimize the energy, as indicated above. The radial functions for SOC are normally represented analytically, e.g. by (normalized) Slater-type orbitals (STO).

The SOC method has been successfully applied to a number of atomic systems, by e.g. Weiss [44], and Hibbert [45]. However, the number of terms needed for a given accuracy with this method can be rather large.

MULTI-CONFIGURATION HARTREE-FOCK

In the *multi-configuration Hartree-Fock* scheme (MCHF) [46], the HForbitals, as well as the extra orbitals, are re-optimized to minimize the energy, E , of the state of interest. The variational method is used in order to determine equations for the radial functions similar to the HF equations (section 4.3). While the radial functions used for SOC are normally analytic, numerical functions are practically always used in the MCHF method. The solution process is iterative, with each iteration consisting of two parts.

Firstly, for a given estimate of the expansion coefficients c_i ($i=1,2,\dots$), the equations are solved self-consistently to obtain radial functions. Secondly, for these radial functions, a new set of c_i coefficients is obtained by solving the matrix-equation (4.17). These steps are repeated, giving successively better and better functions until the desired degree of convergence is obtained.

The MCHF method was used in some of the work presented in this thesis to obtain correlated wavefunctions. The method was then used in a "*frozen core approximation*". For example, in the calculation of Ga wavefunctions, the 1s, 2s, 2p, 3s, 3p and 3d orbitals were determined by a single-configuration HF calculation of the Ga $4s^2 4p^2 P$ ground state. In all the remaining calculations this "core" was kept unchanged, or "frozen", while the motion of the outer electrons was correlated. Radiative transition probabilities and lifetimes in neutral Ga (papers IX and X), and the hyperfine interactions in the lowest 2D states in neutral Al, Ga and In (paper VI) were determined from such wavefunctions.

The MCHF method is very effective at capturing the dominant correlation effect. However, one often encounters difficulties with the method in dealing with a series of weakly interacting states. For example, inclusion of a configuration with one of the inner s-electrons, from a closed s-subshell, excited to a higher n-quantum number, (e.g including $1sns(^1S)2s^2...$ in the expansion of a $1s^2(^1S)2s^2...$ "configuration") normally gives a very small contribution to the total energy being optimized. This kind of *polarization* of closed s-subshells might, however, give large contributions to the magnetic hyperfine interaction through the contact term in Eq. (2.11).

Perturbation theory, on the other hand, has exactly the opposite characteristics - large correlation effects are difficult to incorporate but a large number of small effects can readily be included. The perturbational approach to accurate calculations of hyperfine interactions is presented in the next chapter.

4.7 EFFECTIVE OPERATORS AND PERTURBATION THEORY

Atomic hyperfine structures are measured with high accuracy by the Lund group (papers IV, V and VI in this thesis) and the need for accurate calculations beyond the CFM is therefore obvious. The use of perturbation theory for accurate calculations, going to high orders in the perturbation expansion, requires a systematic approach. The method used in this thesis, and which will be described here, is based on effective operators and a diagrammatic form of *many-body perturbation theory* MBPT [47]. This method can be applied to a large variety of physical interactions. In the work on which this thesis is based, however, MBPT is only used for *ab initio* calculations of atomic hyperfine structures (paper V). In this chapter the method is outlined in the form in which it was used when doing these calculations. It is therefore natural that the idea of effective hyperfine operators be described in the same chapter.

4.7.a EFFECTIVE HYPERFINE OPERATORS

In chapter 2 the hyperfine operators were presented as (2.11 and 2.12)

$$H_{\text{hfi-dipole}} = \alpha^2 \sum_i \left(\frac{1}{r^3} - \sqrt{10} (\mathbf{s} \cdot \mathbf{C}^2)^1 r^{-3} + \frac{8\pi}{3} \mathbf{s} \delta(\mathbf{r}) \right) \mu_I \quad (4.18a)$$

$$H_{\text{hfi-quadrupole}} = -\frac{1}{2} \sum_i \mathbf{C}^2 \mathbf{Q}^2 r^{-3} \quad (4.18b)$$

The summation is performed over all electrons in the system. In a CFM, however, the closed shells give no net contribution, and the summation is limited to open shells.

A CFM, such as restricted HF, often predicts hyperfine interactions in poor agreement with experiment, even if the predictions of the total energies are relatively good. (Examples of this was given on page 27.) This is related to

polarization of the inner, closed shells due to the interaction with the polarized open valence shell, and to the correlated motion of the electrons. One kind of core polarization, often of great importance, is the *spin polarization*, or "*induced contact interaction*". The radial functions for closed shells depend on the m_s quantum number due to exchange interactions with the electrons in the open shell. The hyperfine interactions from the two s-electrons, with opposite spin orientations, therefore do not cancel completely.

There is also an orbital polarization, which is caused by the nonspherical charge distribution of the valence shell. This affects the core electrons differently, depending on their m_l quantum numbers and, as a first approximation, it can be interpreted as a quadrupole distortion of the closed shells. This distortion gives an additional quadrupole interaction with the nucleus, which is known as *the Sternheimer effect* [48].

In *spin-polarized Hartree-Fock* (SPHF) the radial functions for different m_s quantum numbers are allowed to be different, and in the *unrestricted Hartree-Fock* (UHF) model all orbitals are allowed to be different. If a model such as UHF is used, instead of a CFM, the summation in Eq.(4.18) must be carried out over all electrons since the *closed* shells are no longer completely isotropic. One disadvantage with such a procedure is that the contributions from inner shells are obtained as small differences between very large numbers.

An alternative procedure is to replace the "true" hyperfine operator by an "effective" operator which, by definition, operates only within the open shells. Polarization and most of the correlation effect can be included by allowing the radial factors of the orbital, spin-dipole and quadrupole terms for the valence electron to be different. The spin polarization of the closed s-shells, for example, can be represented by a *contact term* for the valence electrons, even when there are no s electrons in the open shells. The effective hyperfine operators then take the following form

$$H_{\text{hfi-dipole}}^{\text{eff}} = \alpha^2 \sum_i \left[(\mathbf{l} \langle r^{-3} \rangle_{\text{orb}} - \sqrt{10} (\mathbf{s} \mathbf{C}^2)^1 \langle r^{-3} \rangle_{\text{s-d}} + \mathbf{s} \langle r^{-3} \rangle_{\text{c}}) \mu_I \right] \quad (4.19a)$$

$$H_{\text{hfi-quadrupole}}^{\text{eff}} = - \frac{1}{2} \sum_i \mathbf{C}^2 \mathbf{Q}^2 \langle \bar{r}^3 \rangle_q \quad (4.19b)$$

where the summation is now limited to the open shells. Experimental hyperfine structures are very well fitted with this type of operator, treating the different radial integrals as free parameters. In the dipole case relativistic effects can also be expressed by means of the same operator, while the quadrupole interaction requires additional terms [49].

4.7.6 MANY-BODY PERTURBATION THEORY

The UHF model contains polarization effects but no correlation between the electrons. To estimate the correlation effects it is therefore necessary to go beyond the independent particle models, and the MCHF method was discussed above. To treat weak interactions in an accurate way, and to make a direct connection with the effective operators discussed above, a perturbational approach is often preferable. Effects beyond UHF involve the correlated motion of

two or more electrons, and represent *pure many-body effects*. When these correlations are included in the perturbational approach, *many-body perturbation theory* is obtained.

In the perturbational approach one starts with a zero-order or "model" Hamiltonian, H_0 , with known eigenvalues and eigenfunctions,

$$H_0 \Psi_0^i = E_0^i \Psi_0^i \quad (i=1,2,3\dots). \quad (4.20)$$

The difference between the "true" and the model Hamiltonian is the perturbation

$$V = H - H_0. \quad (4.21)$$

Frequently a central-field model, such as HF, is used for H_0 and V is then the non-central part of the electrostatic interaction, and other smaller effects such as the hyperfine interaction.

The Hilbert space of the system is partitioned into two parts, a model space (D), spanned by the eigenfunctions of H_0 , and a complementary space (Q). (The model space is often limited to a singel configuration). Two projection operators are formed; P , which projects any wavefunction, Ψ , in the Hilbert space onto the model space, and $Q = 1 - P$, which projects Ψ onto the complementary space. The projections of the true wavefunctions, Ψ^i , onto the model space are called the model functions

$$\Psi_0^i = P \Psi^i \quad (i = 1, 2, 3 \dots d) \quad (4.22)$$

where d is the dimension of the model space.

We also define a *wave operator*, Ω , which transforms the model functions back into the corresponding true wavefunctions

$$\Psi^i = \Omega \Psi_0^i \quad (i = 1, 2, 3 \dots d). \quad (4.23)$$

From the Schrödinger equation

$$H \Psi^i = E^i \Psi^i \quad (4.24)$$

operating with P from the left and using (4.22) and (4.23) gives

$$P H \Omega \Psi_0^i = E^i \Psi_0^i \quad (4.25)$$

$H_{\text{eff}} = P H \Omega$ is called *the effective Hamiltonian* and it satisfies the eigenvalue equation

$$H_{\text{eff}} \Psi_0^i = E^i \Psi_0^i \quad (i = 1, 2, 3 \dots d). \quad (4.26)$$

This means that the exact energies of the states, corresponding to the model states, are obtained by solving the *effective operator equation* (4.26), instead of the full Schrödinger equation (4.24). No approximations have been made so far, the only sacrifice in making this change is that only a limited number (d) of energies are obtained. One should note that the effective Hamiltonian, H_{eff} , is the same for the entire model space. Therefore, if this operator is known with sufficient accuracy, it yields directly the energy structure of all the corresponding states. This is one advantage of this technique over, for instance, the variational procedure, where a separate calculation has to be performed for each state.

When the hyperfine interaction is studied, we add this to the noncentral part of the electrostatic perturbation, $V = V_{\text{es}} + h$, and H_{eff} is separated into two parts, one independent and one dependent on h . The latter part is defined as the effective operator h_{eff} corresponding to the interaction h .

To facilitate the numerical evaluation of the operator h_{eff} , the various contributions to the effective Hamiltonian can be conveniently represented by means of diagrams. The convention for doing this is to represent the orbitals by vertical lines and the interactions by dashed horizontal lines (fig. 4.1). Since this operator acts only within the open shell, the free lines must all be open-shell lines. In an atom with only one electron in an open shell there can only be a one-body operator, with one free valence line at the top and bottom.

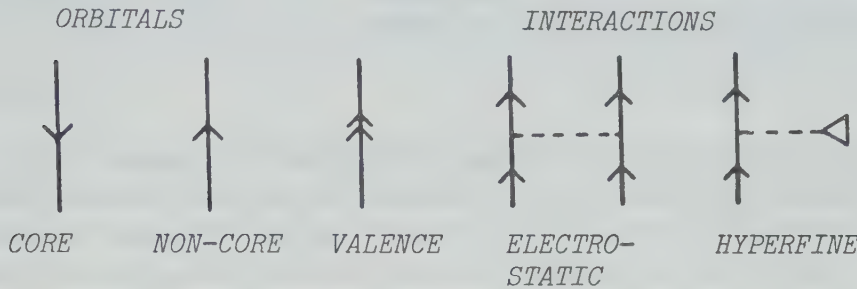


FIG 4.1

By making a perturbation expansion of the wave operator, Ω , and using the *linked-diagram theorem* [50], this operator can be shown to have the following expansion (keeping only terms linear in h)

$$h_{\text{eff}} = \left[h + h \frac{Q}{E_0 - H_0} V + V \frac{Q}{E_0 - H_0} h + h \frac{Q}{E_0 - H_0} V \frac{Q}{E_0 - H_0} V + \right. \\ \left. + V \frac{Q}{E_0 - H_0} h \frac{Q}{E_0 - H_0} V + V \frac{Q}{E_0 - H_0} V \frac{Q}{E_0 - H_0} h + \dots \right]_{\text{linked}} \quad (4.27)$$

where all first-, second- and third-order terms (characterized by the total number of interactions) have been included. (Terms in Ω which are independent of h are omitted since these contribute only to the total *term* splittings but not to the hfs splittings of interest here.) Only "linked" diagrams are included, this means that the diagrams to be evaluated must not have any disconnected, closed parts. For the hyperfine energy contribution to the state Ψ^1 this gives

$$E_h^i = \langle \Psi_0^i | h_{\text{eff}} | \Psi_0^i \rangle = E_h^{i(1)} + E_h^{i(2)} + E_h^{i(3)} + \dots \\ (i = 1, 2, 3, \dots, d) \quad (4.28)$$

The first-order effect is entirely a polarization effect, while the third- (and higher) order effects include electron correlation.

The first-order value of the effective hyperfine operator is represented by the diagram in fig. 4.2a. Polarization diagrams, e.g. the one in fig. 4.2b, are characterized by the fact that there is only one excitation at a time, while correlation diagrams, e.g. fig. 4.2c, contain simultaneous excitations of several electrons. (There are 66 different correlation diagrams in the third order.)

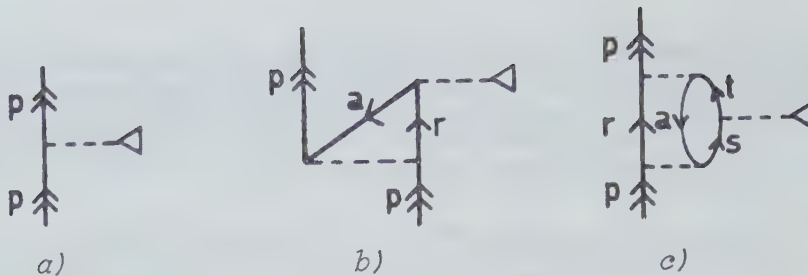


FIG 4.2

As an illustration of the evaluation of a diagram consider the exchange polarization diagram in fig. 4.2b. For example, the large polarization effect of the closed core in the Ga 4p $^2P_{3/2}$ state (paper V and table 4.1 below) is represented by this diagram, and it has the value

$$\sum_{a,r} \langle a|h|r \rangle \langle pr | \frac{1}{r_{12}} | ap \rangle / (\epsilon_a - \epsilon_r) \quad (4.29)$$

where the summation is performed over all a = core orbitals (a stands for $n_a l_a$), and r = excited orbitals. Each term in the summation can be separated into a radial and an angular (and spin) part. The angular part of the diagram can be reduced and evaluated using *angular momentum graphs* [51]. The diagram above can be written, after reduction of the angular momentum graph

$$\text{Diagram} = R (-1)^x \left\{ \begin{matrix} l_p & x & l_p \\ l_a & k & l_r \end{matrix} \right\} \times \text{Diagram} \quad (4.30)$$

where R is a radial factor, $\{ \}$ is a 6-j symbol, and k and κ are the ranks of the interactions. Similarly, it can be shown that, as in the case illustrated here, all diagrams of an effective one-body operator can be expressed as a numerical factor times the same first-order diagram. But this means that all these diagrams can be represented by an operator having the same tensorial structure as the true operator and operating only on the unperturbed functions.

All higher order effects are simply included in the multiplicative constant. This is the idea behind the effective operators. The radial factor as well as the 6-j symbol in the expression (4.30) depends on the tensor rank of the operator, and this explains how the $\langle r^{-3} \rangle$ parameters of the different terms in the effective operator become different.

The exchange polarization diagram discussed above contains the "radial part"

$$\sum_{a,r} \frac{\langle n_a l_a || h || n_r l_r \rangle R^k(n_p l_p n_r l_r, n_a l_a n_p l_p) (-1)^k \langle l_p || C^k || l_a \rangle \langle l_r || C^k || l_p \rangle}{\epsilon_{n_a l_a} - \epsilon_{n_r l_r}} \quad (4.31)$$

The summation over core orbitals (a) is finite, but the summation over excited orbitals (r) is infinite and also includes continuum states. This factor can be evaluated using two essentially different methods. Firstly, a "complete" set of single-particle states (ϕ_i , $i=1,2,\dots$), including unbound states, of H_0 is generated, and the necessary summation and integration are then performed. This was the method used by Kelly [52] for instance, in his early work on atomic many-body calculations.

The other technique, which is used in this thesis, is based on the solution of an inhomogeneous, differential equation satisfied by the "wave package" appearing in the expression for the diagram, Eq. (4.31). By performing the summation over n_r separately, a *single-particle function* (spf) is obtained

$$\rho^k(n_a l_a \rightarrow l_r; r) = \sum_{\substack{n_r \\ (\text{non-core})}} \frac{P_{n_r l_r}^{(r)} R^k(n_p l_p n_r l_r, n_a l_a n_p l_p)}{\epsilon_{n_a l_a} - \epsilon_{n_r l_r}} \quad (4.32)$$

Eq. (4.31) can now be reduced to

$$\sum_{n_a l_a l_r k} (-1)^{k < l_p} |c^k| |l_a > l_r |c^k| |l_p > n_a l_a |h| |\rho^k(n_a l_a \rightarrow l_r) > \quad (4.33)$$

where the infinite sum over n_r is removed. The infinite sum appears instead in the expression for the spf, and at first sight no simplification is obtained. However, it can be shown [53] that the spf satisfies an inhomogeneous differential equation. The spf can therefore be obtained by solving a differential equation - a *single-particle equation*. The need to generate a complete set of excited orbitals, and to perform the infinite summation is thereby eliminated.

The single-particle equation may be solved a number of times, once for each excitation $n_a l_a \rightarrow l_r$ being considered. The same spf can be used to evaluate the corresponding contribution to the other terms of the hyperfine operator, as only the integral in Eq. (4.33) will be dependent on the rank of the particular operator.

By solving single-particle equations iteratively, higher order polarization diagrams are included (c.f. fig. 4.3a). When calculating core polarization effects in neutral Ga (paper V) the single particle equations were solved iteratively until self-consistency was obtained. In this way core-polarization effects were essentially evaluated to all orders of perturbation theory.

Similarly, diagrams with double excitations, e.g. the one in fig. 4.2c, are evaluated by means of a two-dimensional *pair function*

$$\rho^k(n_p l_p \rightarrow l_r, n_a l_a \rightarrow l_t; r_1 r_2) \quad (4.34)$$

The two-particle pair equation is considerably more complicated to solve than the single-particle equation described above. There are, however, several techniques available [54]. The pair equations can, just as the single-particle equation, be solved iteratively [55]. In the work on Ga mentioned above, however, only first-order pair functions were evaluated. By combining first-order spf and pair functions all third-order hyperfine effects can be evaluated, but since the spf's are evaluated to all orders, important higher order effects are automatically included. In the Ga calculation some of the higher order effects were also included by the modifications of the HF orbitals towards Brueckner orbitals, e.g. by the diagram in fig. 4.3b.

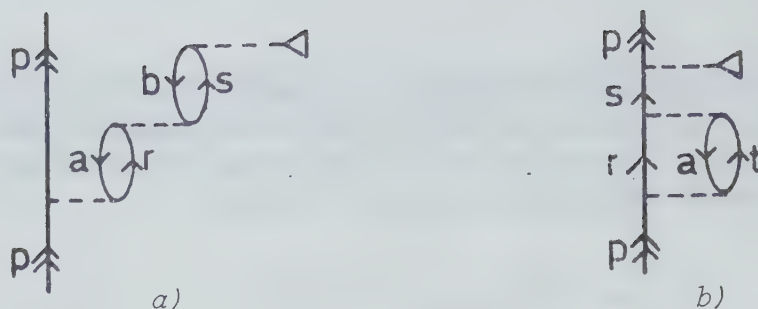


FIG 4.3

All the numerical work on MBPT presented in this thesis was done using computer programs developed and kindly communicated by the Chalmers group [56].

As examples of results obtained with MBPT, A factors for the 2P ground states of Li (calculated from values in [57]) and Ga (paper V) are given in table 4.1.

Table 4.1

	Li 2p	$A(^2P_{1/2})$	$A(^2P_{3/2})$	Ga 4p	$A(^2P_{1/2})$	$A(^2P_{3/2})$
Hartree-Fock		32.30	6.47		975.5	195.1
Polarization		11.59	-10.58		201.6	-169.5
Correlation		2.31	0.79		11.8	161.0
Relativistic effects		---	---		162.8	2.0
Total (MBPT)		46.20	-3.32		1351.7	188.6
Experimental		45.91	-3.06		1338.99	190.79

The core polarization can obviously have a considerable effect on the atomic hyperfine interaction. It is entirely responsible for the inversion of the hyperfine splitting in the lowest Li 2P state. The unrestricted Hartree-Fock model, which contains polarization effects but no correlation, would also be able to reproduce this inversion, but a central-field model (e.g. HF) gives erroneous results. For the Ga4p 2P state, however, UHF would not be an appropriate method, since the polarization and correlation effects are of the same magnitude but have different signs. Including polarization effects, but no correlation would, in this case, give results far from the experimental ones.

It is apparently important to include polarization as well as correlation in accurate calculations of atomic hyperfine interactions. The above MBPT approach is well suited to this kind of calculation if the correlation effects are not too large. In a current project [58], the hyperfine interactions in the $3s^23d$ 2D states of neutral aluminum are being studied with the MBPT approach.

The preliminary results for the $^2D_{5/2}$ state, for instance, indicate that the all-order polarization effects, starting from $3s^23d$, adds -5 MHz to the first order A factor (0.4 MHz), and the first order correlation effect adds +8 MHz. To treat these heavily perturbed states to the same order in the perturbation expansion as the Ga np^2P states in paper V is apparently not sufficient since the experimentally obtained value for $A(^2D_{5/2})$ is 185 ± 5 MHz (paper VI).

By solving the pair functions and generating approximate Brueckner orbitals iteratively, the contribution to the contact interaction from the $3s3d \rightarrow pp$ pair function increases by more than one order of magnitude. The A factor for the $^2D_{5/2}$ state increases at the same time to about 120 MHz. However, still only about 2/3 of the experimental value is reproduced, and further effects must be accounted for. Therefore, in paper VI, the MCHF method was instead employed for this calculation. In the MCHF approach the large contribution from the $3s3d \rightarrow pp$ pair function is represented by a large mixing coefficient for the $3s3p^2$ term in the expansion of the " $3s^23d \ ^2D$ " state. As mentioned on p 33, however, weakly interacting configurations, representing, e.g, core polarization, are not as accurately accounted for with the MCHF method as with MBPT.

Starting the MBPT calculations from an *extended but incomplete model space* [59] is an alternative approach considered for the Al case discussed above [58]. This might be the ideal choice for accurate calculations of heavily perturbed states. In this approach the perturbation expansion starts from a linear combination of configurations, such as $c_1 3s^23d + c_2 3s3p^2$ for the Al 2D states discussed above. In this way the dominant correlation effects can be taken into account already in a first-order calculation and polarization of the core from the $3s3p^2$ configuration is included in a second-order calculation. (Starting from $3s^23d$ this polarization appears first in the fifth order of the perturbation expansion.)

4.8 THE COULOMB APPROXIMATION

A frequently used *semi-empirical* method for the determination of transition probabilities and lifetimes, is the *Coulomb approximation* (CA). It has a rather simple structure, and the computational effort required for each transition probability is considerably less than that required for more elaborate methods, such as MCHF. Experimental lifetimes in the literature are often compared with values obtained with the CA. Therefore, even if this method has not been used for the calculations presented in this thesis, it will be outlined briefly here, partly to motivate the use in this thesis of the more time-demanding MCHF method.

The essential use of the CA is to evaluate the radial functions needed in the evaluation of the transition integrals. The CA is a one-electron approximation, so correlation effects are not included explicitly. Bates and Damgaard [60] demonstrated numerically in the late 1940's, that often only the region of r where the potential is, say, within 1% of its asymptotic Coulomb form, contributes significantly to the radial transition integral. This suggests replacing the radial wave equation by

$$\left[-\frac{1}{2} \frac{d}{dr} + \frac{l(l+1)}{2r^2} - \frac{Z_{\text{net}}}{r} - \epsilon_j \right] P_j(r) = 0 \quad (4.45)$$

where Z_{net} is the net charge of the ionic core, and ϵ_j is the orbital energy given by the effective principal quantum number n^* derived from the *observed* energies. The solutions to this equation are hydrogenic wavefunctions with the non-integral principal number n^* . (Bates and Damgaard used analytic functions in their early work.)

As the ϵ_j 's are normally not eigenvalues of equation (4.45), the solution may diverge at the origin. The integration of the equation must therefore be cut off at some finite radius, and the normalization will be an uncertain part of this approximation. Clearly, the CA is best suited for radial functions for high-lying Rydberg states of alkay-like systems. To evaluate the lifetimes, however, transition integrals involving radial functions for low-lying states are also required, and then the above approximation is rather crude.

The approximation can be improved by adding some kind of model potential correction $V(r)$ to account for some of the non-coulombic contribution from the core. This can be included in equation (4.45) simply by making the effective charge r -dependent, $Z_{\text{net}} \rightarrow Z_{\text{net}}(r)$. The radial functions are then obtained by starting at infinity and integrating the equation numerically inwards to the cut-off radius. This is the *numerical Coulomb approximation* (NCA)[61]. More elaborate modifications are sometimes used, for example, when the radial functions are required to pass through zero at the origin [62].

It should be apparent that the results obtained with the MCHF method, used in this thesis, are more reliable than those obtained by the CA or NCA described above. This is especially true whenever correlation effects have an important influence on the radiative transition probabilities, as is the case in, for example, the 2D sequence in Ga (papers IX and X), and whenever there is more than one electron in an open shell involved in the transition. However, the amount of effort required in the calculations is also worth mentioning. The computing time per matrix element, using the NCA is of the order of only a few seconds [61]. The corresponding time using the MCHF method, including the time needed for selecting a proper representation of each state, amounts to days or even weeks.

5 COMMENTS ON THE PAPERS

The papers on which this thesis is based are all results of extensive team work. Several people have contributed to varying extents in different parts of the work presented. In this chapter some comments will be made concerning my part in the different investigations, and some reflexions will be made on the results.

Papers I-III

The spectrum of Sr V, The spectrum of Rb IV and Revised and extended analysis of Xe III

My contribution in these three papers has been in the interpretation of the experimentally obtained energy levels. In none of the investigations have I taken any part in the experiments.

The analysis of the Sr V spectrum, was my first analysis of this kind, using the method described in section 4.4. A large part of the time was devoted to the search for an explanation of the large deviation between the observed and calculated positions of the 3S_1 level in the lowest p^3d configuration. Corresponding deviations had previously been observed in Ne III, Na IV, Mg V and in the Rb IV spectrum being investigated in parallel (paper II). The introduction of Rydberg series interactions in the interpretation of the p^3d configurations was found to account for most of the 3S_1 deviation in Sr V and at the same time improve the overall fit. The effects of Rydberg series interactions are normally not considered in the analyses found in the literature, but were in this analysis found to play an important role. This kind of interaction was therefore also included in the analyses of the Rb IV and Xe III spectra (papers II and III) and found to have the same effect there as well. This is probably one of the more important theoretical observations made in these investigations.

In a recently published study [63] of the Y VI spectrum, Rydberg series configuration-interaction was not included in the theoretical interpretation. The deviation between observed and calculated positions for the lowest p^3d 3S_1 level was found to be very large ($\sim 3000 \text{ cm}^{-1}$) and therefore excluded from the least-squares fit.

The analysis of the Xe III spectrum includes classification of observed laser lines and an interpretation of Xe $N_{4,5}00$ Auger spectra.

Paper IV

Natural radiative lifetimes and hyperfine structure in the $4s^26p$ $^2P_{3/2,1/2}$ levels of gallium

Chronologically this is my first paper, and the project where I devoted most time to the experimental part of the investigation. The semiempirical analysis of the observed hyperfine structure was rather simple. The observations concerning the sign and significance of core polarization, however, were later found to be consistent with corresponding observations based on more elaborate theoretical calculations (paper V).

Paper V

Experimental and theoretical studies in the $4s^2np\ ^2P$ sequence of neutral gallium

A large portion of my time has been devoted to the MBPT approach for accurate calculations. The work has included program implementation, test runs and calculations which are still in progress [58,64]. However, of the ten papers on which this thesis is based, this paper is the only one where MBPT has been used. This was the first time this particular approach was applied to atoms in this region of the periodic table, and to facilitate the use of computer programs originally designed for alkali-like systems, the two 4s electrons were treated as being part of the closed core, and the p electron as a single valence electron. The results presented in the paper clearly demonstrate the applicability of this approach to three-electron systems such as Ga $4s^2np$.

Paper VI

Hyperfine structure studies in 2D and 4P states of ^{27}Al , $^{69,71}Ga$ and ^{115}In

The work presented in this paper can be separated into two parts with respect to the authors: Zhao and Lundberg performed the hyperfine structure measurements and Carlsson and I did the theoretical analysis. The calculations presented were not performed to obtain very accurate *ab initio* values, but rather to indicate the origin of the extremely large deviations between the experimental results obtained for the lowest nd 2D states and the corresponding single-configuration Hartree-Fock values. (As discussed in chapter 4.7, these deviations are being investigated further in a current project [58] using the MBPT approach.) In the paper it is also shown for ^{115}In , that the $sp^2\ ^4P$ states are well represented by a single configuration model, but that relativistic effects play an important role in the hyperfine structures in an element as heavy as In.

Paper VII

Hyperfine-dependent lifetimes induced by singlet-triplet mixing

The results presented in this paper are rather unique as this is the first time that lifetimes dependent on the F-quantum numbers have been observed using laser-spectroscopic techniques. Experimentally this was a challenge, and high spectral and temporal resolution were required simultaneously. My part in this investigation was mainly on the theoretical side. Before the experiment was performed, and after the first measurements of the unperturbed lifetimes, theoretical estimates were made in order to indicate the magnitude of the expected effect. In this way the experimental set-up could be optimized. After the measurements were completed, the results were interpreted in terms of the hyperfine-induced singlet-triplet mixing of different substates.

Paper VIII

Natural radiative lifetimes in the 1P_1 and 1F_3 sequences of Sr I

In this study I took part in the experimental work, but spent most of the time on the interpretation of the results obtained.

The lifetimes obtained for the $5s6p$, $5s7p$ and $5s8p$ 1P_1 states are about one order of magnitude longer than values previously reported in the literature. The trend of the lifetimes indicates further that these states are strongly perturbed.

The lowest 1F_3 state, belonging to the doubly excited $4d5p$ configuration, was found to have a very long lifetime compared with the lowest $5snf$ 1F_3 state even though very strong mixing between these states had been reported. The lifetimes in the rest of the $5snf$ 1F_3 sequence appeared to scale close to the n^{*3} law for unperturbed Rydberg sequences.

The interpretation of the experimental results would obviously have benefitted from theoretical *ab initio* calculations. However, this is one of my earliest papers, and was completed before I had initiated my collaboration with C. Froese Fischer and learned how to perform MCHF calculations of lifetimes. This is reflected in the lack of theoretical calculations presented in this paper.

During the last two years extensive MCHF investigations of the experimental results reported in this paper have been performed in Brussels and Amsterdam [65]. These calculations (not yet completed) indicate at least two interesting results. Firstly, the observed perturbation in the $5snp$ 1P_1 sequence, giving rise to the long lifetimes at the beginning of the sequence, is well reproduced by the *ab initio* calculations, and the lifetimes are found to be in good agreement with our results.

Secondly, the results indicate that the 1F_3 sequence is *not* unperturbed, but that the $4d5p$ 1F_3 perturber strongly affects the lifetimes of the whole $5snf$ 1F_3 Rydberg series. The fact that the lifetimes scale close to the n^{*3} law is therefore "accidental".

Papers IX and X

Experimental and theoretical investigation of radiative lifetimes in neutral gallium and Lifetimes and oscillator strength trends for the $4s^2nd$ 2D series of Ga I

These papers are the result of an initial desire to investigate the influence of the $4s4p^2$ 2D perturber on the lifetimes of the nd 2D states in neutral gallium, and, at the same time, test the MCHF approach for lifetime calculations in an element as heavy as Ga. However, in the course of this investigation the theoretical as well as the experimental side of the project increased. Extensive MCHF calculations were performed to obtain accurate wavefunctions, and the experimental investigation was extended to include lifetimes of 2P and 2S states. The results were finally presented as two separate papers.

Paper IX presents the experimental investigation and the results of the MCHF calculations. In paper X, which is the only "theoretical" paper in this thesis, the interaction between the non-localized sp^2 perturber and the nd 2D Rydberg series is treated in detail, in particular the importance of the position of the perturber relative to the unperturbed series.

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7 REFERENCES

1. L.I. Schiff, *Quantum Mechanics*, Ch 13, McGraw-Hill, 1968
2. Appendix A in Ref. 47
3. A. Messiah, *Quantum Mechanics*, North-Holland, 1961
4. M. Blume, A.J. Freeman and R.E. Watson, *Phys.Rev.*, A134, 320 (1964)
5. Ch II.3 in: I. Lindgren and A. Rosén, *Case Stud. At. Phys.*, 4, 93 (1974)
6. Ch 8.29 in: I.I. Sobel'man, *Introduction to the Theory of Atomic Spectra*, Pergamon Press, 1972
7. K.J. Kollath and M.C. Standage, Ch 21 in: Hanle and Kleinpoppen (eds.), *Progress in Atomic Spectroscopy*, Plenum Press, 1979
8. Ch. 14 and 15 in: R.D. Cowan, *The Theory of Atomic Structure and Spectra*, University of California Press, 1981
9. J.Y.C. Chen, *J. Chem. Phys.*, 40, 615 (1964)
10. Sect. 5.1.4 in: A. Hibbert, *Rep. Prog. Phys.*, 38, 1217 (1975)
11. R.A. Sawyer, *Experimental Spectroscopy*, Dover Publications, 1963.
12. S.G. Pettersson, *Phys. Scr.*, 21, 296 (1982)
13. I. Martinsson, *Nucl. Instr. Meth.*, 202, 1 (1982)
14. S.P. Sumner, *Diffraction Grating Spectrographs*, Holt-Rinehart-Winston, 1970
15. Ch. 3 in: W. Demtröder, *Laser Spectroscopy*, Springer, 1982
16. H. Rinneberg, J. Neukammer, G. Jönsson, H. Hieronymus, A. König and K. Vietzke, *Phys. Rev. Lett.*, 55, 382 (1985)
17. S. Svanberg, *Atomic and Molecular Spectroscopy*, Springer-Verlag (in preparation)
18. Ch. 10 and 11 in Ref. 15 and K. Shimoda (ed.), *High Resolution Laser Spectroscopy*, Topics in Applied Physics, Vol. 13, Springer-Verlag, 1976
19. M.J. Colles and C.P. Pidgeon *Rep. Prog. Phys.*, 38, 329, (1975) and Ch. 5-7 in Ref. 15
20. M.S. Soren and A.L. Schawlow, *Opt. Commun.*, 5, 148 (1972) and J.L. Hall *IEEE J. QE.*, 4, 638 (1968) and J.L. Hall and J.A. Magyar in Ref. 18 "High Resolution..." and

Ch 10.2 in Ref. 15

21. S.C. Wieman and T.W. Hänsch Phys. Rev. Lett., 36, 1170 (1976) and
Ch. 10.3 in Ref 15
22. G. Grynberg and B. Cacnac Rep. Prog. Phys., 40, 791 (1977)
23. J.N. Dodd and G.W. Series, Ch. 14 in: Hanle and Kleinpoppen (eds.), *Progress in Atomic Spectroscopy*, Plenum Press, 1978
24. Ch. 7.5 in Ref. 15
25. P.A. Franken, Phys. Rev., 121, 508 (1961)
26. R.E. Imhof and F.H. Read, Rep. Prog. Phys., 40, 1, (1977)
27. Ch. 15 in: A. Corney, *Atomic and Laser Spectroscopy*, Clarendon Press, Oxford, 1977
28. M. Gustavsson, H. Lundberg, L. Nilsson and S. Svanberg, J. Opt. Soc. Am., 69, 984 (1979)
29. Ch. 2 in Ref. 15
30. Ch. 4.5 in Ref. 15
31. A. R. Edmonds, *Angular Momentum in Quantum Mechanics*, Princeton Univ. Press, 1960 and
U. Fano and G. Racah, *Irreducible Tensorial Sets*, Academic Press, 1959 and
Ch. 11 in Ref. 15.
32. Ch. 2 in Ref. 46 and
Ch. 6 and 12 in Ref. 15
33. Ch 8.6 in: D. Park, *Introduction to the Quantum Theory*, McGraw-Hill, 1974
34. Ch. XIE in: C. Cohen-Tannoudji, B. Diu and F. Laloë, *Quantum Mechanics*, John Wiley & Sons, 1977
35. Ch. 17.6 in: G. Arfken, *Mathematical Methods for Physicists*, Academic Press, 1970
36. Ch. 7 in Ref. 47
37. C. Froese Fischer, Comput. Phys. Commun., 4, 107 (1972) and
C. Froese Fischer, DOE Report No. DOE/ER/10618-11 (1983)
38. Ch. 7 in Ref. 15
39. E.U. Condon and G.H. Shortley, *The Theory of Atomic Spectra*, Cambridge University Press, 1935

40. J.H. Wilkinson, *The Algebraic Eigenvalue Problem*, Clarendon Press, 1965
41. The matrix elements were calculated and the energy matrixes diagonalized using computer programs developed by R.D. Cowan, see Ch. 16 in Ref. 15
42. Ch. 16 in Ref. 15
43. Ch. 2.5 in Ref. 46
44. A.W. Weiss, Phys. Rev., 122, 1826 (1961)
A.W. Weiss, Phys. Rev., A9, 1524 (1974)
45. A. Hibbert, J. Phys. B, 7, 1417 (1974) *and*
A. Hibbert, P.L. Dufton, M.J. Murray, D.G. York, Mon. Not. R. Astron. Soc. , 205, 535 (1984)
46. C Froese Fischer, *The Hartree-Fock Method for Atoms*, John Wiley and sons, 1977
47. I. Lindgren and J. Morrison, *Atomic Many-Body Theory*, Springer Series in Chemical Physics 13, Springer-Verlag, 1982
48. R.M. Sternheimer, Phys. Rev., A6, 1702 (1972)
49. Ch. II.5 in: I. Lindgren and A. Rosén, Case Stud. At. Phys., 4, 93 (1974)
50. Ch. 12.5.2 in Ref. 47
51. Ch. 3 and 4 in Ref. 47
52. H.P. Kelly, Phys. Rev. 131, 684 (1963)
53. Ch. 13.5.1 in Ref. 47
54. A.-M. Mårtensson, J. Phys. B, 12, 3995 (1979) *and*
V. McKoy and N.M. Winter, J. Chem. Phys. 48, 5514 (1968)
55. Ref. 54 and: I. Lindgren Phys. Rev., A31, 1273 (1985)
56. Ref. 55 and: S. Garpman, I. Lindgren, J. Lindgren and J. Morrison, Z. Physik, A276, 167 (1976)
57. I. Lindgren Phys. Rev., A31, 1273 (1985)
58. I. Lindgren, S. Salomonson and C.-G. Wahlström, Work in progress (*Hyperfine interactions in perturbed 2D states in Al and Ga*)
59. I. Lindgren and D. Mukherjee, Submitted to Physics Reports
60. D.R. Bates and A. Damgaard, Phil. Trans. R. Soc., A242, 101 (1949)
61. A. Lindgård and S.E. Nielsen, J. Phys. B, 8, 1183 (1975)

62. C.E. Theodosiou, Phys. Rev., A30, 2881 (1984)
63. W. Persson and J. Reader, J. Opt. Soc. Am., B3, 959 (1986)
64. J.L. Heully, S. Salomonson, and C.-G. Wahlström, Work in progress (*Hyperfine structures of Cu, Ag and Au 2P levels*)
65. M. Godefroid and J.E. Hansen, Private Communication

PAPER I

Spectrum of SrV

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Abstract

The spectrum of four-times ionized strontium has been observed in the 2500–200 Å range. About 650 lines have been classified as transitions between 95 odd levels belonging to the $4s4p^5$, $4s^24p^35s$, $6s$, $4d$ and $5d$ configurations and 43 even levels belonging to the $4s^24p^4$, $4s^24p^35p$, $4f$ and $5f$ configurations. The observed level structure has been interpreted by means of Hartree–Fock calculations and parametric fits. It is suggested that a systematic discrepancy between observed and predicted positions of the 3S term in p^3d configurations is due to Rydberg-series configuration interaction.

1. Introduction

The quadruply ionized strontium atom, Sr^{4+} , is isoelectronic with neutral selenium. The ground configuration of Sr V is $4s^24p^4$ while the lower excited configurations are $4s4p^5$, $4s^24p^34d$ and $4s^24p^35s$. The first study of this spectrum was reported in 1974 by Hansen and Persson [1], who reported the levels of the ground configuration and the $4s4p^5$ configuration.

The present study is based on an observation of the sliding-spark spectrum of strontium in the 9800–200 Å range. About 650 Sr V lines have been classified as transitions between 95 odd levels belonging to the $4s4p^5$, $4s^24p^35s$, $6s$, $4d$ and $5d$ configurations and 43 even levels belonging to the $4s^24p^4$, $4s^24p^35p$, $4f$ and $5f$ configurations.

For all configurations but $4f$ and $5f$ the observed energy-level structure has been compared with the results of theoretical calculations including configuration-interaction effects. In the $4f$ and $5f$ configurations only the 5F terms have been established.

2. Experimental

The strontium spectrum was excited in a sliding-spark discharge [2]. The fifth spectrum was well developed at a peak value of the discharge current of 1000 A.

No Sr V lines could be identified above 2500 Å. In the 2500–430 Å range the spectrum was recorded on a 3 m normal-incidence spectrograph [3] having a plate factor of 2.77 Å mm^{-1} in the first diffraction order. A 5 m grazing-incidence spectrograph [4] was used to photograph the spectrum in the 500–200 Å range. The plate factor of this instrument varies from 0.62 Å mm^{-1} at 500 Å to 0.42 Å mm^{-1} at 200 Å.

The wavelengths and intensities of all classified Sr V lines are given in Tables I and II. The intensity figures are visual estimates of photographic density. The uncertainty in the wavelength determinations in the normal-incidence region is 0.02 Å above 2000 Å and 0.01 Å below this limit. In the grazing-incidence region the measured wavelength values are accurate to 0.005 Å . However, very few impurity lines useful as reference lines are present on the grazing-incidence exposures, and in some wavelength regions, in particular for the shortest wavelengths, Sr V

Ritz standards (see below) had to serve as complementary reference lines.

All experimentally established Sr V levels are given in Tables III and IV. The level values of the $4p^3nl$ states were determined using a least-squares procedure which takes the observed wavenumbers, weighted according to their estimated uncertainty, into account. The internal consistency of the $4p^3nl$ level system is estimated to be $\pm 0.2 \text{ cm}^{-1}$. Many downward transitions from $4d$ and $5s$ states were observed in higher diffraction orders of the normal-incidence spectrograph, thus providing an accurate determination of the excited configurations relative to the ground configuration. On an absolute scale the level values are correct to $\pm 1 \text{ cm}^{-1}$. From these level values it is possible to calculate accurate wavelengths for the transitions from the levels of the $5s$, $6s$, $4d$ and $5d$ configurations to the levels of the ground configuration. These calculated wavelengths, which are given in the last column of Table II, are accurate to 0.003 Å around 600 Å and to 0.0005 Å around 220 Å. Calculated wavelengths of about the same precision have previously been reported for Sr III [2] and Sr IV [5]. Table V is a compilation of the proposed strontium reference lines.

3. Analysis

When establishing the energy levels we were guided by theoretical predictions of the structures of the configurations. The predictions were obtained by diagonalizing the energy matrices with appropriately scaled Hartree–Fock (HF) values for the energy parameters. (All HF calculations have been performed with the Froese–Fischer computer program [6].) For the odd configurations effects of configuration interaction were taken into account by treating the $4s4p^5 + 4s^24p^3 (nd + (n+1)s)$ configurations together.

The analysis started by using the levels of the ground configuration [1] to establish $J = 0–3$ levels of the odd configurations. These odd levels were then used to locate the levels of the $5p$ configuration which, in turn, were used to extend the $4d$, $5d$, $5s$ and $6s$ levels to higher J values.

Figure 1 shows the relative positions and extensions of the investigated configurations. Almost all levels of the $4s^24p^4$, $4s4p^5$, $4s^24p^35s$, $6s$, $5p$, $4d$ and $5d$ configurations have been experimentally established, whereas in the $4f$ and $5f$ configurations only levels based on the 4S parent term have been located.

The coupling conditions in all investigated $4s^24p^3nl$ configurations of Sr V show an intermediate character and the choice of coupling scheme is more or less arbitrary. For the sake of conformity we have chosen to use the LS coupling scheme throughout this report.

3.1. Odd configurations

When interpreting the $4d + 5s$ configurations the $J = 1$ levels in

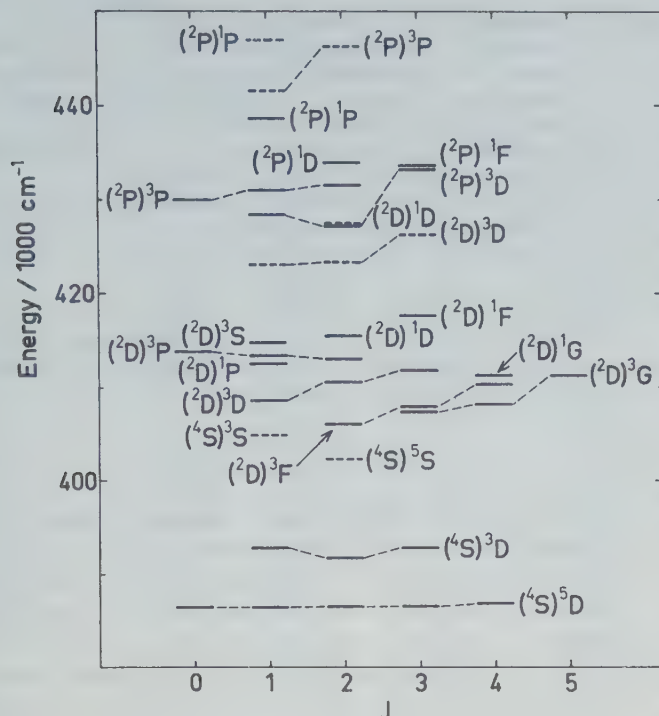


Fig. 3. Structure of the $4s^2 4p^3(5d + 6s)$ configurations of Sr V. $5d$ levels are indicated by fully drawn lines, $6s$ levels by dashed lines. All levels are designated in the LS coupling scheme.

$5d4p$), $R^1(4p4d, 6d4p)$ and $R^1(4p5d, 6d4p)$), were kept fixed at their Hartree-Fock ratios. Taken together this means that only four fully adjustable parameters have been introduced to account for all interactions.

The level distribution in the $4d + 5s$ and $5d + 6s$ configurations is shown in Figs. 2 and 3. The observed positions of the nd levels are indicated by fully drawn lines whereas the positions of the ns levels are indicated by dashed lines. Table VI gives the results of the least-squares fit of the energy parameters to the observed levels as described above. The resulting parameter values are given in Table VII.

A fit to the $4s4p^5 + 4s^24p^3(4d + 5s)$ levels gives a mean error of the order of 800 cm^{-1} while in a corresponding fit to the $4s4p^5 + 4s^24p^3(5d + 6s)$ levels the mean error is approximately 250 cm^{-1} . A fit to the $4s4p^5 + 4s^24p^3(4d + 5d + 5s + 6s)$ levels neglecting the Rydberg-series interactions gives a mean error of about 500 cm^{-1} with, evidently, the major part of the error arising in the $4d$ configuration. This latter number should be compared with the mean error in the final fit including series interaction (Tables VI and VII) which amounts to 391 cm^{-1} .

One reason for including the Rydberg-series configuration interaction in the theoretical interpretation was the large discrepancy between the observed and calculated positions of the $(^2D)4d\ ^3S_1$ level. This discrepancy decreases from over 3000 cm^{-1} to less than 1000 cm^{-1} by the inclusion of the series interaction. Simple perturbation calculations indicate that relative term shifts of the order of 4000 cm^{-1} might occur as a result of the series interaction. However, it seems difficult to completely disentangle the large specific discrepancy of the 3S_1 level. It might be related to the size of the $G^1(4p, 4d)$ energy parameter (which gives a large diagonal contribution to the energy of the 3S state). In a calculation neglecting the series interaction the fitted value of G^1 is $55\,300\text{ cm}^{-1}$ (scaling factor 0.76) whereas

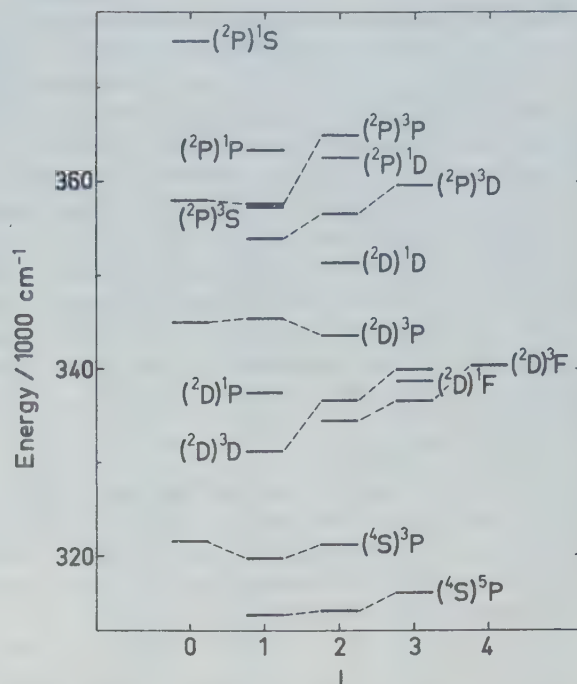


Fig. 4. Structure of the $4s^2 4p^3 5p$ configuration of Sr V. The levels are designated in the LS coupling scheme.

in the final fit G^1 has increased to $60\,400\text{ cm}^{-1}$ (scaling factor 0.83). This increase in G^1 roughly corresponds to the improvement in the fit to the 3S_1 level.

It appears that those $4d$ terms that have the largest diagonal $g_1 \cdot G^1$ matrix elements, namely $(^2P)^1P$ ($g_1 = +0.700$), $(^2D)^1F$ ($g_1 = +0.600$) and $(^2D)^1D$ ($g_1 = +0.500$) are just those states which, according to a simple perturbation calculation, are most affected (depressed) by the $4d \rightleftharpoons 5d$ series interaction. In a calculation neglecting series interactions the effects of the $4d \rightleftharpoons 5d$ interaction might be absorbed by $G^1(4p, 4d)$, resulting in a small fitted value of G^1 . The $(^2D)^3S$ term which also has a large diagonal $g_1 \cdot G^1$ matrix element ($g_1 = +0.467$), is much less affected by the series interaction ($\approx 1000 \text{ cm}^{-1}$ as compared with $3\text{--}4000 \text{ cm}^{-1}$). The reason for the large discrepancy between the observed and calculated level values of the $(^2D)4d^3S$ term should thus be that this term is relatively unperturbed.

The second largest discrepancy between observed and calculated level values in the $4d$ configuration in a single-configuration calculation is found for the $(^2D)^1S_0$ level (the corresponding discrepancy is also present in Rb IV [7]). This discrepancy is not affected by the inclusion of the $4d \leftrightarrow 5d$ interaction. This is not surprising in the light of the discussion above: the $(^2D)^1S$ state is not only relatively unaffected by the series interaction but also, unlike the $(^2D)^3S$ state, has only a minor diagonal $g_1 \cdot G^1(4p, 4d)$ matrix element.

To ensure that the reduction of the mean error of the least-squares fit including the Rydberg-series interaction is not only a consequence of the improved fit for the $(^2D)4d^3S$ term another set of calculations was performed in which the 3S_1 level was excluded from the fit. Also in this case the introduction of the series interaction contributes to a substantial reduction in the mean error, from about 420 cm^{-1} to about 350 cm^{-1} , i.e., to an improvement of the overall fit.

One specific consequence of the introduction of the series interaction is that the designations of the two accidentally close-lying levels at $291\,678\text{ cm}^{-1}$ ($((2D)4d^1F_3)$) and $291\,836\text{ cm}^{-1}$

((²D)5s³D₃) become interchanged. According to Table VI the levels are heavily mixed whereas a calculation neglecting the series interaction identifies the lower level as an almost 100% pure (²D)5s³D₃ level. Although this latter result is in agreement with an "experimental" classification based on combination properties we have chosen to retain the classifications according to the series-interaction calculation. The reason for the ambiguity should not be considered as a deficiency in the series-interaction calculation as such (when using HF values for the series-interaction integrals the levels are "correctly" identified) but rather as a more general problem in least-squares fits to observed structures involving close-lying levels belonging to different configurations.

3.2. Even configurations

The ground configuration has been discussed in detail previously [1]. Figure 4 shows the level distribution in the 4s²4p³5p configuration while the results of fitting the energy parameters to the observed levels are given in Table VIII. The fitted parameter values compare well with HF values (Table IX).

The results given in Tables VIII and IX are from a single-configuration calculation. Inclusion of the effective configuration-interaction parameter, α , results in a slightly better fit than the one quoted, the mean error decreasing from 171 to 165 cm⁻¹. The 4s²4p⁴ ↔ 4s²4p³5p interaction does not seem to have any major influence on the level distribution in the 5p configuration.

The average purity of the 5p levels in the LS coupling scheme is 70%. It appears that the true coupling conditions in the 5p configuration are best approximated by the LS scheme. However, for several levels the largest eigenvector component is less than 50%.

The (⁴S)4f⁵F levels have been determined from combinations with 4d in the 540 Å range. The centres of gravity of the 4s²4p³4f and 4s4p⁴4d configurations are estimated to be roughly coincident. Consequently the two configurations will interact strongly, making an extended analysis of the 4f configuration very complicated. The (⁴S)5f⁵F levels given in Table III have been determined from combinations with both 4d and 5d. However, based on quantum-defect arguments the identification of the levels as 5f levels is somewhat questionable.

4. Ionization energy

The ionization energy of Sr V has been estimated from a comparison of the quantum defects in the *ns* and *nd* series of Sr V and Sr IV. The value obtained is 570 000 ± 5000 cm⁻¹. This value of the ionization energy leads to a reasonable value of the quantum defect for the (⁴S)4f⁵F term but to a too small quantum defect for the (⁴S)5f⁵F term. As already pointed out this observation casts some doubt on the identification of the even levels around 458 000 cm⁻¹ as (⁴S)5f⁵F levels.

Acknowledgements

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References

1. Hansen, J. E. and Persson, W., J. Opt. Soc. Am. 64, 696 (1974).
2. Persson, W. and Valind, S., Physica Scripta 5, 187 (1972).

3. Minnhagen, L., Physica Scripta 11, 38 (1975).
4. Lundström, T. and Minnhagen, L., Physica Scripta 5, 243 (1972).
5. Hansen, J. E. and Persson, W., Physica Scripta 13, 166 (1976).
6. Froese Fischer, C., Comput. Phys. Commun. 4, 107 (1972).
7. Persson, W. and Wahlström, C. -G., Work in progress.
8. Artru, M. -C. and Kaufman, V., J. Opt. Soc. Am. 70, 1130 (1980).
9. Persson, W. and Di Rocco, O., Work in progress.
10. Cowan, R. D., The theory of Atomic Structure and Spectra, Ch. 13. University of California Press (1981).
11. Radziemski, L. J., Jr. and Kaufman, V., J. Opt. Soc. Am. 64, 366 (1974).
12. Hansen, J. E. and Persson, W., Work in progress.
13. When calculating matrix elements, diagonalizing energy matrices and performing least-squares fits the computer programs developed by R. D. Cowan have been used. See [10], Ch. 16.

Table I. Observed combinations between excited states of Sr V. Abbreviations for line characteristics: a = affected (by); bl = blended (by); h = hazy; u = unsymmetrical; w = wide. Intensities are uncorrected visual estimates of the photographic densities of the lines. All levels are given in LS notation. A calculated wavenumber given with only one decimal indicates that the level value of one of the levels involved in the transition has been determined from this line alone

Intensity and shape	λ_{vac} (Å)	σ (cm ⁻¹)		Classification
		Obs.	Calc.	
9	2 376.333	42 081.7	.58	(² D)5s ³ D ₂ -(² D)5p ³ D ₁
10	2 360.349	42 366.6	.62	(² D)5s ³ D ₁ -(² D)5p ³ D ₁
10	2 345.430	42 636.1	.15	(² D)5s ¹ D ₂ -(² D)5p ¹ P ₁
8	2 342.666	42 686.4	.46	(² D)4d ¹ F ₃ -(² D)5p ³ F ₂
m Sr III		42 818.	.42	(² P)5s ¹ P ₁ -(² P)5p ³ P ₁
6	2 324.866	43 013.2	.28	(⁴ S)4d ³ D ₂ -(⁴ S)5p ³ P ₁
15	2 279.273	43 873.6	.69	(² D)5s ¹ D ₂ -(² D)5p ¹ F ₃
6	2 254.962	44 346.6	.61	(² D)4d ¹ P ₁ -(⁴ S)5p ³ P ₁
0.5	2 251.357	44 417.7	.59	(⁴ S)4d ³ D ₂ -(⁴ S)5p ³ P ₂
0.5	2 228.806	44 867.1	.08	(² P)5s ³ P ₂ -(² P)5p ³ D ₂
12	2 228.010	44 883.1	.00	(⁴ S)5s ³ S ₁ -(⁴ S)5p ³ P ₁
12	2 224.944	44 944.9	.86	(² D)4d ¹ F ₃ -(² D)5p ³ F ₃
12	2 216.704	45 112.0	.03	(² D)5s ¹ D ₂ -(² D)5p ³ D ₃
12	2 210.039	45 248.1	.21	(² D)5s ³ D ₂ -(² D)5p ³ F ₂
10	2 196.194	45 533.3	.25	(² D)5s ³ D ₁ -(² D)5p ³ F ₂
10	2 195.475	45 548.2	.15	(² P)5s ³ P ₂ -(² P)5p ³ S ₁
10	2 185.750	45 750.9	.92	(² D)4d ¹ P ₁ -(⁴ S)5p ³ P ₂
m Sr III		45 854.	.61	(² P)5s ³ P ₂ -(² P)5p ³ P ₁
9	2 172.102	46 038.4	.30	(² P)5s ³ P ₁ -(² P)5p ³ D ₁
15	2 160.422	46 287.3	.31	(⁴ S)5s ³ S ₁ -(⁴ S)5p ³ P ₂
10	2 156.293	46 375.9	.91	(² D)4d ³ P ₂ -(⁴ S)5p ³ P ₁
10	2 141.836	46 688.9	9.07	(⁴ S)5s ³ S ₁ -(⁴ S)5p ³ P ₀
9	2 137.113	46 792.1	.15	(² D)4d ³ P ₂ -(⁴ S)5p ⁵ P ₂
8	2 134.187	46 856.2	.27	(² D)5s ³ D ₃ -(² D)5p ¹ F ₃
10	2 127.051	47 013.5	.43	(² D)4d ¹ F ₃ -(² D)5p ¹ F ₃
9 w	2 116.975	47 237.2	.35	(² P)5s ³ P ₀ -(² P)5p ³ D ₁
15	2 109.634	47 401.6	.61	(⁴ S)5s ⁵ S ₂ -(⁴ S)5p ⁵ P ₁
9	2 101.796	47 578.4	.33	(² D)5s ³ D ₂ -(² D)5p ³ D ₂
12 bl Sr IV	2 094.220	47 750.5	.83	(² P)5s ¹ P ₁ -(² P)5p ¹ D ₂
7	2 093.392	47 769.4	.35	(² P)4d ¹ P ₁ -(² P)5p ³ D ₁
15	2 091.269	47 817.9	.85	(⁴ S)5s ⁵ S ₂ -(⁴ S)5p ⁵ P ₂
12	2 089.282	47 863.3	.37	(² D)5s ³ D ₁ -(² D)5p ³ D ₂
9	2 088.116	47 890.1	.06	(² D)5p ¹ F ₃ -(⁴ S)5d ⁵ D ₂
12	2 085.634	47 947.1	.20	(² P)5s ³ P ₂ -(² P)5p ³ D ₃
10	2 072.468	48 251.6	.77	(² D)4d ¹ F ₃ -(² D)5p ³ D ₃
3	2 058.298	48 583.8	.83	(² D)5s ³ D ₃ -(² D)5p ³ F ₄
9	2 057.773	48 596.2	.30	(² D)5s ¹ P ₁ -(² P)5p ¹ P ₁
10	2 056.655	48 622.6	.68	(² D)5s ³ D ₁ -(² D)5p ¹ P ₁
15	2 051.662	48 741.0	0.99	(² D)4d ¹ F ₃ -(² D)5p ³ F ₄
12	2 050.847	48 760.3	.38	(² P)5s ³ P ₁ -(² P)5p ³ D ₂
3	2 050.642	48 765.2	.11	(² D)5s ¹ D ₂ -(² D)5p ³ P ₂

Table I. Continued

Intensity and shape	$\lambda_{\text{vac.}}$ (Å)	σ (cm ⁻¹)		Classification
		Obs.	Calc.	
m 2 × Sr III		48 768.	.87	(² D)4d ³ P ₂ -(⁴ S)5p ⁵ P ₃
12	2017.136	49 575.2	.18	(² D)5s ³ D ₂ -(² D)5p ¹ F ₃
10	2010.504	49 738.8	.86	(⁴ S)4d ³ D ₃ -(⁴ S)5p ³ P ₂
3	2010.133	49 747.9	.91	(² P)5s ³ P ₁ -(² P)5p ³ P ₁
15	2008.248	49 794.6	.57	(⁴ S)5s ⁵ S ₂ -(⁴ S)5p ⁵ P ₃
6	1993.990	50 150.7	.61	(² P)5s ¹ P ₁ -(² P)5p ³ P ₂
7	1991.242	50 219.9	.92	(² D)4d ³ P ₁ -(⁴ S)5p ³ P ₁
6	1989.291	50 269.2	.18	(² P)5s ³ P ₁ -(² P)5p ³ P ₀
5	1980.541	50 491.3	.43	(² P)4d ¹ P ₁ -(² P)5p ³ D ₂
6	1969.008	50 787.0	.02	(² P)5s ³ P ₂ -(² P)5p ¹ D ₂
12	1967.972	50 813.7	.52	(² D)5s ³ D ₂ -(² D)5p ³ D ₃
10	1962.826	50 947.0	6.96	(² P)5s ³ P ₀ -(² P)5p ³ P ₁
6	1937.074	51 624.3	.23	(² D)4d ³ P ₁ -(⁴ S)5p ³ P ₂
15	1926.598	51 905.0	4.85	(² D)4d ¹ F ₃ -(² D)5p ³ P ₂
12	1880.162	53 186.9	.80	(² P)5s ³ P ₂ -(² P)5p ³ P ₂
1	1839.024	54 376.7	.78	(⁴ S)4d ³ D ₂ -(² D)5p ³ D ₁
8	1835.993	54 466.4	.60	(² D)5s ³ D ₂ -(² D)5p ³ P ₂
2	1829.633	54 655.8	.92	(² D)4d ³ S ₁ -(⁴ S)5p ³ P ₁
m Sr III		54 680.	.32	(² P)5s ³ P ₁ -(² P)5p ¹ D ₂
9	1821.041	54 913.6	.72	(⁴ S)5s ⁵ S ₂ -(⁴ S)5p ³ P ₂
6	1800.964	55 525.8	.79	(² P)5s ³ P ₁ -(² P)5p ¹ P ₁
7	1789.786	55 872.6	.25	(² P)5p ¹ S ₀ -(² P)5d ³ P ₁
5	1780.579	56 161.5	.50	(² D)5p ³ D ₂ -(⁴ S)5d ³ D ₃
m Sr V		56 225.	.72	(² D)5s ³ D ₁ -(² D)5p ³ P ₀
7 a Sr II	1778.492	56 227.4	.56	(² D)5s ³ D ₂ -(² D)5p ³ P ₁
6	1777.885	56 246.6	.50	(⁴ S)5s ³ S ₁ -(² D)5p ³ P ₁
2	1772.694	56 411.3	.37	(² P)4d ¹ P ₁ -(² P)5p ¹ D ₂
0.5	1771.093	56 462.3	1.99	(² D)4d ³ S ₁ -(⁴ S)5p ³ P ₀
7 a	1769.524	56 512.4	.60	(² D)5s ³ D ₁ -(² D)5p ³ P ₁
12	1769.311	56 519.2	.32	(² D)5s ¹ D ₂ -(² D)5p ¹ D ₂
m Sr III		56 642.	.20	(² D)5p ¹ D ₂ -(² D)5d ³ F ₃
0.5	1746.515	57 256.9	.84	(² P)4d ¹ P ₁ -(² P)5p ¹ P ₁
1	1737.818	57 543.4	.41	(⁴ S)4d ³ D ₂ -(² D)5p ³ F ₂
5	1694.147	59 026.8	.60	(² D)5s ¹ D ₂ -(² P)5p ³ D ₁
4	1676.188	59 659.2	.06	(² D)4d ¹ F ₃ -(² D)5p ¹ D ₂
10 a Al II	1670.173	59 874.0	3.53	(⁴ S)4d ³ D ₂ -(² D)5p ³ D ₂
4	1669.621	59 893.9	4.18	(² D)4d ¹ D ₂ -(² D)5p ³ P ₁
9	1655.182	60 416.3	.22	(² P)5s ¹ P ₁ -(² P)5p ¹ S ₀
2 h	1631.451	61 295.1	.04	(² D)5p ³ P ₂ -(⁴ S)6s ³ S ₁
6	1623.813	61 583.4	.42	(² D)4d ³ P ₁ -(² D)5p ³ D ₁
5 a Sr IV	1616.275	61 870.7	.38	(⁴ S)4d ³ D ₂ -(² D)5p ¹ F ₃
7	1613.779	61 966.4	.17	(² D)4d ¹ P ₁ -(² D)5p ¹ P ₁
3 Sr V?	1607.189	62 220.4	.81	(² D)5s ³ D ₂ -(² D)5p ¹ D ₂
m Sr III		62 502.	.56	(⁴ S)5s ³ S ₁ -(² D)5p ¹ P ₁
0.5	1593.973	62 736.3	.21	(² D)5s ¹ D ₂ -(² P)5p ³ P ₁
4	1590.713	62 864.9	.68	(⁴ S)4d ³ D ₃ -(² D)5p ³ F ₂
7 a Sr IV	1574.093	63 528.6	.74	(² D)5p ³ P ₀ -(² D)5d ³ D ₁
4	1573.306	63 560.4	.42	(² P)5p ¹ S ₀ -(² P)5d ¹ P ₁
9	1557.519	64 204.7	.86	(² D)5p ¹ D ₂ -(² D)5d ¹ D ₂
10 bl 2 × Sr IV	1541.099	64 888.8	.42	(² D)4d ¹ F ₃ -(² P)5p ³ D ₂
9	1534.389	65 172.5	.65	(² D)5p ³ P ₁ -(² D)5d ³ D ₂
4	1533.866	65 194.7	.80	(⁴ S)4d ³ D ₃ -(² D)5p ³ D ₂
4	1531.926	65 277.3	.13	(⁴ S)4d ³ D ₁ -(² D)5p ³ P ₁
9 a	1530.364	65 344.0	3.63	(² P)4d ³ D ₂ -(⁴ S)5p ⁵ P ₁
5	1529.330	65 388.1	.14	(⁴ S)5p ³ P ₂ -(⁴ S)5d ⁵ D ₃
3	1520.685	65 759.9	.87	(² P)4d ³ D ₂ -(⁴ S)5p ⁵ P ₂
9	1517.734	65 887.7	.43	(² D)4d ¹ D ₂ -(² D)5p ¹ D ₂
4	1514.713	66 019.1	.42	(² D)4d ³ S ₁ -(² D)5p ³ D ₁
10	1507.832	66 320.4	.35	(² D)5p ¹ D ₂ -(² D)5d ¹ F ₃
0.5	1498.494	66 733.7	.74	(⁴ S)5p ³ P ₁ -(⁴ S)5d ⁵ D ₁
5	1497.862	66 761.8	.80	(⁴ S)4d ³ D ₂ -(² D)5p ³ P ₂
7	1496.690	66 814.1	3.94	(² P)5p ³ P ₂ -(² P)5d ³ P ₂
7 a Sr IV	1492.213	67 014.6	3.84	(² D)4d ³ P ₂ -(² D)5p ³ F ₂
0.5	1489.363	67 142.8	.14	(² D)5p ³ P ₁ -(² D)5d ¹ P ₁
8	1483.043	67 428.9	9.02	(² D)5p ³ P ₀ -(² D)5d ¹ P ₁
6	1477.792	67 668.5	.62	(² D)5s ¹ D ₂ -(² P)5p ¹ D ₂
0.5	1474.677	67 811.5	.38	(² D)5s ³ D ₃ -(² P)5p ³ D ₃
6	1474.527	67 818.4	.38	(² D)5p ³ F ₄ -(² D)5d ³ G ₄

Table I. Continued

Intensity and shape	$\lambda_{\text{vac.}}$ (Å)	σ (cm ⁻¹)		Classification
		Obs.	Calc.	
4	1474.069	67 839.4	.48	(² D)4d ³ P ₁ -(² D)5p ¹ P ₁
9	1471.259	67 969.0	8.54	(² D)4d ¹ F ₃ -(² P)5p ³ D ₃
9 bl	1468.390	68 101.8	2.04	(² D)5p ³ P ₁ -(² D)5d ³ P ₁
9	1465.909	68 217.0	6.88	(² D)5p ³ P ₂ -(² D)5d ³ D ₃
4	1463.786	68 316.0	.27	(² P)5p ³ P ₂ -(² P)5d ³ D ₃
6	1462.669	68 368.2	.25	(² P)5p ¹ P ₁ -(² P)5d ³ P ₂
7 a Sr V	1462.068	68 396.3	4.71	(² D)4d ¹ D ₂ -(² P)5p ³ D ₁
6	1461.181	68 437.8	.70	(² D)5s ³ D ₂ -(² P)5p ³ P ₁
5	1460.322	68 478.1	.20	(² D)5p ³ P ₁ -(² D)5d ³ P ₀
4	1459.546	68 514.5	.09	(² D)5s ¹ D ₂ -(² P)5p ¹ P ₁
9	1459.367	68 522.9	.76	(⁴ S)4d ³ D ₂ -(² D)5p ³ P ₁
2	1457.926	68 590.6	.58	(² D)5p ¹ F ₃ -(² D)5d ³ G ₃
10	1457.054	68 631.6	.52	(⁴ S)5s ³ S ₁ -(² D)5p ³ P ₂
8	1456.140	68 674.7	.81	(² D)5p ¹ P ₁ -(² D)5d ³ F ₂
9	1454.041	68 773.9	.80	(² P)5p ³ P ₂ -(² P)5d ¹ F ₃
2	1451.307	68 903.4	.10	(² D)5p ³ P ₂ -(² D)5d ¹ P ₁
7	1450.980	68 919.0	.21	(⁴ S)4d ³ D ₃ -(² D)5p ³ F ₄
2	1447.776	69 071.5	.64	(² P)5p ³ P ₂ -(² P)5d ¹ D ₂
6	1447.667	69 076.7	.76	(² P)4d ¹ P ₁ -(² P)5p ¹ S ₀
1	1445.540	69 178.3	.19	(² P)4d ³ F ₂ -(⁴ S)5p ³ P ₁
2	1445.374	69 186.2	.05	(² D)4d ³ S ₁ -(² D)5p ³ F ₂
8	1443.581	69 272.2	.24	(² D)4d ³ P ₂ -(² D)5p ³ F ₃
5	1442.090	69 343.8	.96	(² D)4d ³ P ₂ -(² D)5p ³ D ₂
9	1440.412	69 424.6	.49	(² D)5p ³ P ₂ -(² D)5d ³ P ₂
0.5	1438.721	69 506.2	5.84	(² D)5p ³ F ₃ -(² D)5d ³ F ₂
9	1437.898	69 546.0	5.94	(² D)5p ¹ F ₃ -(² D)5d ³ G ₄
7	1435.693	69 652.8	.89	(² P)5p ³ P ₁ -(² P)5d ³ D ₁
7	1435.487	69 662.8	.70	(² P)5p ³ P ₁ -(² D)6s ¹ D ₂
4 a	1431.520	69 855.8	6.09	(² D)4d ¹ P ₁ -(² D)5p ³ P ₁
4	1430.225	69 919.1	8.81	(² D)4d ³ P ₀ -(² D)5p ³ P ₁
10	1429.677	69 945.9	.94	(² D)5p ³ F ₃ -(² D)5d ³ F ₄
5 a C III	1426.519	70 100.7	3.27	(² D)4d ³ P ₂ -(² D)5p ¹ P ₁
0.5	1425.515	70 150.1	.44	(² P)4d ³ D ₁ -(⁴ S)5p ⁵ P ₁
7	1420.852	70 380.3	.29	(² P)5p ³ P ₀ -(² P)5d ³ D ₁
7 a 2 × Sr IV	1420.609	70 392.4	.48	(⁴ S)5s ³ S ₁ -(² D)5p ³ P ₁
10 bl Sr IV	1419.752	70 434.8	5.16	(² D)5p ³ D ₃ -(² D)5d ³ F ₄
8	1419.204	70 462.0	.00	(⁴ S)5p ⁵ P ₃ -(⁴ S)5d ⁵ D ₂
10	1418.292	70 507.3	.29	(⁴ S)5p ⁵ P ₃ -(⁴ S)5d ⁵ D ₃
9	1417.759	70 533.8	.77	(⁴ S)5p ³ P ₂ -(⁴ S)5d ³ D ₂
9	1416.687	70 587.2	6.69	(² D)5p ³ D ₃ -(² D)5d ³ D ₂
8	1415.902	70 626.3	5.95	(² D)5p ³ D ₂ -(² D)5d ³ G ₃
2	1415.616	70 640.6	.42	(² P)5p ¹ P ₁ -(² P)5d ¹ D ₂
m Sr V		70 650.	.23	(² P)5p ³ D ₂ -(² D)6s ¹ D ₂
10	1415.402	70 651.3	.20	(² D)5s ³ D ₃ -(² P)5p ¹ D ₂
9 bl 3 × Sr IV	1415.274	70 657.7	9.15	(² D)5p ³ F ₃ -(² D)5d ³ G ₃
9	1414.101	70 716.3	.05	(² P)5p ¹ D ₂ -(² P)5d ³ D ₃
15	1413.882	70 727.3	.27	(⁴ S)5p ⁵ P ₃ -(⁴ S)5d ⁵ D ₄
12	1412.958	70 773.5	.5	(² D)5p ³ F ₄ -(² D)5d ³ G ₅
0.5	1412.259	70 808.5	.36	(² D)4d ¹ F ₃ -(² P)5p ¹ D ₂
2	1410.405	70 901.6	.56	(² P)5p ³ P ₁ -(² P)5d ³ D ₁
9	1407.120	71 067.2	.00	(⁴ S)5p ³ P ₀ -(⁴ S)5d ³ D ₁
9	1405.019	71 173.4	.58	(² P)5p ¹ D ₂ -(² P)5d ¹ F ₃
10 bl 2 × O III	1404.658	71 191.7	.83	(² D)5p ³ P ₂ -(² D)5

Table I. Continued

Intensity and shape	$\lambda_{\text{vac.}}$ (Å)	σ (cm ⁻¹)		Classification
		Obs.	Calc.	
7 a Sr III, IV	1 391.397	71 870.2	69.96	(² D)5p ³ D ₃ -(⁴ S)5d ³ D ₃
12	1 390.086	71 938.0	.08	(⁴ S)5p ³ P ₁ -(⁴ S)5d ³ D ₂
6	1 386.962	72 100.1	.22	(⁴ S)5d ⁵ D ₄ -(⁴ S)5f ⁵ F ₅
2	1 386.879	72 104.4	.32	(² D)4d ¹ D ₂ -(² P)5p ³ P ₁
9	1 380.732	72 425.4	.30	(⁴ S)5p ⁵ P ₂ -(⁴ S)5d ⁵ D ₁
10	1 380.478	72 438.7	.72	(⁴ S)5p ⁵ P ₂ -(⁴ S)5d ⁵ D ₂
8	1 380.217	72 452.4	.42	(² P)4d ¹ F ₃ -(² D)5p ¹ F ₃
10	1 380.051	72 461.1	.00	(² D)5p ¹ F ₃ -(² D)5d ¹ G ₄
m Al III		72 484.	.01	(⁴ S)5p ⁵ P ₂ -(⁴ S)5d ⁵ D ₃
7	1 377.804	72 579.3	.15	(² D)4d ³ P ₂ -(² D)5p ³ D ₃
8	1 373.669	72 797.7	.75	(⁴ S)5p ⁵ P ₁ -(⁴ S)5d ⁵ D ₀
15 a Sr III	1 372.838	72 841.8	.54	(⁴ S)5p ⁵ P ₁ -(⁴ S)5d ⁵ D ₁
9	1 372.592	72 854.9	4.96	(⁴ S)5p ⁵ P ₁ -(⁴ S)5d ⁵ D ₂
			5.74	(² P)4d ³ D ₂ -(⁴ S)5p ³ P ₂
9	1 372.252	72 872.9	3.07	(⁴ S)5p ³ P ₁ -(⁴ S)5d ³ D ₁
m Sr III, IV		72 917.	.55	(² D)5p ³ F ₂ -(² D)5d ³ G ₃
5	1 368.678	73 063.2	2.57	(² D)5p ¹ P ₁ -(² D)5d ³ D ₂
1	1 368.399	73 078.1	7.57	(² D)5p ¹ D ₃ -(² D)5d ³ P ₂
12	1 365.985	73 207.2	8.14	(² D)4d ¹ F ₃ -(² P)5p ³ P ₂
0.5	1 362.948	73 370.4	.11	(² D)5s ³ D ₂ -(² P)5p ¹ D ₂
m Sr IV		73 470.	.05	(² P)5p ³ P ₁ -(² P)5d ³ P ₁
8	1 359.511	73 555.9	.87	(² P)5p ³ D ₃ -(² P)5d ³ D ₃
7 a Sr IV	1 358.426	73 614.6	.80	(² D)5p ³ F ₂ -(² D)5d ³ F ₃
9 a Sr IV	1 356.095	73 741.2	2.07	(² D)5p ³ F ₃ -(² D)5d ³ F ₄
10	1 355.461	73 775.6	6.51	(² P)5p ³ S ₁ -(² P)5d ³ P ₁
9	1 354.620	73 821.5	.88	(² D)5p ³ D ₂ -(² D)5d ³ D ₃
9	1 351.928	73 968.4	.44	(² D)4d ³ P ₁ -(² D)5p ³ P ₂
8 bl Sr IV	1 351.106	74 013.4	.40	(² P)5p ³ D ₃ -(² P)5d ¹ F ₃
4	1 345.619	74 315.2	.91	(² D)5p ¹ F ₃ -(² D)5d ³ P ₂
8	1 343.139	74 452.5	.59	(² P)5p ³ S ₁ -(² P)5d ³ P ₂
7	1 341.992	74 516.1	.01	(⁴ S)4d ³ D ₂ -(² D)5p ¹ D ₂
8	1 341.752	74 529.4	.57	(² D)5p ³ D ₃ -(² D)5d ¹ G ₄
3	1 340.284	74 611.1	.17	(² P)5p ³ D ₁ -(² P)5d ³ D ₁
m C II		74 930.	.87	(² D)5p ³ D ₁ -(² D)5d ³ F ₂
8	1 332.772	75 031.6	2.06	(² D)5p ¹ P ₁ -(² D)5d ¹ P ₁
8 a Sr III	1 331.440	75 106.7	5.15	(² D)5p ³ D ₂ -(² D)5d ³ D ₃
8	1 330.199	75 176.7	.87	(² D)5p ³ F ₃ -(² D)5d ³ D ₃
2	1 326.606	75 380.3	.34	(² P)5p ¹ P ₁ -(² P)5d ¹ P ₁
2	1 322.536	75 612.3	.15	(² D)5p ³ D ₃ -(² D)5d ¹ D ₂
4	1 320.489	75 729.5	.40	(² D)4d ³ P ₁ -(² D)5p ³ P ₁
1	1 318.047	75 869.8	.78	(² D)5p ¹ D ₂ -(² P)5d ³ D ₂
4	1 317.874	75 879.8	.59	(² D)5p ¹ D ₂ -(² D)6s ¹ D ₂
2	1 315.924	75 992.3	1.96	(² D)5p ¹ P ₁ -(² D)5d ³ P ₁
5	1 313.163	76 152.0	.00	(² D)5p ³ F ₂ -(² D)5d ³ D ₂
8	1 311.331	76 258.4	.24	(² P)4d ³ D ₁ -(⁴ S)5p ³ P ₁
1	1 309.442	76 368.4	.12	(² D)5p ¹ P ₁ -(² D)5d ³ P ₀
8	1 309.154	76 385.2	4.48	(² D)5p ³ F ₃ -(² D)5d ³ P ₂
			5.73	(⁴ S)5s ³ S ₁ -(² D)5p ¹ D ₂
0.5	1 307.190	76 499.9	.74	(⁴ S)4d ³ D ₁ -(² P)5p ³ D ₂
0.5	1 302.906	76 751.5	.27	(² D)5p ³ D ₂ -(² D)5d ³ P ₁
4	1 295.654	77 181.1	0.81	(⁴ S)4d ³ D ₁ -(² P)5p ³ S ₁
6	1 294.366	77 257.9	.93	(⁴ S)5s ⁵ S ₂ -(² D)5p ³ P ₂
9 a Sr IV	1 292.191	77 387.9	.84	(² D)5p ³ D ₁ -(² D)5d ³ D ₁
2 a 3 × Sr IV	1 290.546	77 486.6	7.27	(⁴ S)4d ³ D ₁ -(² P)5p ³ P ₁
8	1 283.984	77 882.6	.20	(² D)4d ¹ D ₂ -(² P)5p ¹ P ₁
2	1 282.514	77 971.9	.57	(² D)5p ³ P ₁ -(² D)6s ³ D ₂
7	1 281.911	78 008.6	.54	(⁴ S)4d ³ D ₁ -(² P)5p ³ P ₀
0.5	1 281.227	78 050.2	.19	(² D)5p ³ P ₀ -(² D)6s ³ D ₁
7	1 280.994	78 064.4	.31	(² P)4d ³ D ₁ -(⁴ S)5p ³ P ₀
6	1 280.601	78 088.3	.03	(² D)5p ¹ P ₁ -(² D)5d ¹ D ₂
10 a Sr IV	1 275.431	78 404.9	.44	(² D)4d ³ S ₁ -(² D)5p ³ P ₂
7	1 266.369	78 965.9	.98	(² D)5p ¹ F ₃ -(² D)5d ¹ F ₃
4	1 264.520	79 081.4	.39	(² D)5p ³ F ₂ -(² D)5d ³ P ₁
5	1 252.542	79 837.7	.28	(⁴ S)4d ³ D ₃ -(² D)5p ¹ D ₂
2	1 243.628	80 409.9	10.22	(² D)5p ³ F ₂ -(² D)5d ³ S ₁
5	1 243.371	80 426.5	.44	(⁴ S)4d ³ D ₂ -(² P)5p ³ S ₁
8	1 238.651	80 733.0	2.90	(⁴ S)4d ³ D ₂ -(² P)5p ³ P ₁
4	1 222.166	81 822.0	.49	(² D)4d ³ P ₀ -(² P)5p ³ S ₁

Table I. Continued

Intensity and shape	$\lambda_{\text{vac.}}$ (Å)	σ (cm ⁻¹)		Classification
		Obs.	Calc.	
2	1 210.831	82 587.9	.50	(² D)4d ¹ P ₁ -(² P)5p ³ P ₀
3	1 208.691	82 734.1	.02	(² D)5p ³ P ₂ -(² D)6s ³ D ₃
4	1 207.514	82 814.8	.93	(² P)4d ³ D ₂ -(² D)5p ³ D ₁
7 bl 2 × O III	1 195.612	83 639.2	.25	(⁴ S)5p ³ P ₂ -(⁴ S)6s ³ S ₁
4	1 164.174	85 897.8	.88	(² D)5p ³ F ₄ -(² D)6s ³ D ₃
2	1 163.039	85 981.6	.56	(² P)4d ³ D ₂ -(² D)5p ³ F ₂
4	1 159.599	86 236.7	.69	(⁴ S)5p ⁵ P ₃ -(⁴ S)6s ⁵ S ₂
0.5	1 141.260	87 622.4	1.74	(² P)4d ³ D ₁ -(² D)5p ³ D ₁
1 u	1 132.347	88 312.1	1.68	(² P)4d ³ D ₂ -(² D)5p ³ D ₂
0.5 a	1 089.684	91 769.8	8.70	(⁴ S)5p ³ P ₂ -(² D)5d ³ P ₂
3	1 088.030	91 909.3	.29	(² D)5p ³ D ₁ -(² D)6s ³ D ₁
0.5	1 087.524	91 952.0	.41	(² D)5p ³ F ₂ -(² D)6s ³ D ₃
0.5	1 086.146	92 068.7	9.08	(² D)4d ³ S ₁ -(² P)5p ³ S ₁
3	1 076.756	92 871.5	.95	(² D)5d ³ P ₁ -(² P)5p ¹ D ₂
4	1 073.897	93 118.8	.49	(² P)4d ³ D ₁ -(² D)5p ³ D ₂
5	1 070.817	93 386.7	.36	(⁴ S)4d ³ D ₃ -(² P)5p ³ P ₂
7	1 070.577	93 407.6	.53	(² P)4d ¹ F ₃ -(² P)5p ³ D ₃
3	1 069.103	93 536.3	.04	(⁴ S)5p ³ P ₂ -(² D)5d ³ S ₁
2	1 068.251	93 611.0	.52	(⁴ S)5p ³ P ₁ -(² D)5d ³ P ₁
4	1 066.652	93 751.3	.56	(² D)5d ³ F ₃ -(⁴ S)5p ⁵ P ₃
8	1 065.209	93 878.3	7.80	(² P)4d ³ D ₁ -(² D)5p ¹ P ₁
1	1 060.409	94 303.2	.28	(⁴ S)5p ³ P ₂ -(² D)5d ¹ D ₂
6	1 056.108	94 687.3	.67	(² P)4d ³ F ₂ -(² D)5p ³ P ₁
0.5	1 050.430	95 199.2	.95	(² P)4d ³ D ₂ -(² D)5p ³ P ₂
10	1 041.936	95 975.2	4.83	(² P)4d ¹ D ₂ -(² D)5p ¹ P ₁
1	1 041.466	96 018.5	.82	(² D)5d ³ P ₁ -(² D)6s ¹ D ₂
9	1 038.991	96 247.2	.35	(² P)4d ¹ F ₃ -(² P)5p ¹ D ₂
0.5	1 033.509	96 757.8	.75	(² D)4d ³ D ₁ -(⁴ S)5p ⁵ P ₁
10	1 031.343	96 961.0	0.91	(² P)4d ³ D ₂ -(² D)5p ³ P ₁
8	1 030.441	97 045.8	.46	(² P)4d ³ P ₁ -(² D)5p ³ P ₀
9 bl?	1 027.408	97 332.4	.34	(² D)5d ³ P ₁ -(² D)5p ¹ D ₂
10	1 020.437	97 997.2	.04	(² P)4d ³ D ₃ -(² D)5p ¹ D ₂
8	1 020.001	98 039.1	.01	(² D)4d ³ D ₃ -(⁴ S)5p ⁵ P ₂
7	1 015.736	98 450.8	.71	(² P)4d ¹ D ₂ -(² D)5p ³ D ₃
10	1 013.711	98 647.4	.13	(² P)4d ¹ F ₃ -(² P)5p ³ P ₂
8	1 011.419	98 871.0	0.71	(² D)4d ³ F ₃ -(⁴ S)5p ³ P ₂
7	1 007.198	99 285.3	.02	(² D)4d ³ F ₂ -(⁴ S)5p ³ P ₁
6	1 002.933	99 707.6	.73	(² D)4d ³ S ₁ -(² P)5p ³ P ₂
5	1 000.567	99 943.4	.12	(² D)4d ³ D ₂ -(⁴ S)5p ⁵ P ₁
4	999.846	100 015.4	.73	(² D)4d ³ D ₃ -(⁴ S)5p ⁵ P ₃
0.5	996.419	100 359.4	.36	(² D)4d ³ D ₂ -(⁴ S)5p ⁵ P ₂
7	993.232	100 681.4	0.92	(² P)4d ³ F ₂ -(² D)5p ¹ D ₂
4	993.152	100 689.5	.33	(² D)4d ³ F ₂ -(⁴ S)5p ³ P ₂
5	985.718	101 448.9	.30	(² P)4d ³ P ₂ -(² P)5p ³ D ₂
8	985.408	101 480.8	.84	(² P)4d ³ D ₁ -(² D)5p ³ P ₀
6	982.630	101 767.7	.72	(² P)4d ³ D ₁ -(² D)5p ³ P ₁
5	981.929	101 840.3	.70	(² D)4d ¹ G ₄ -(² D)5p ³ F ₃
2	979.661	102 076.2	.74	(⁴ S)5p ³ P ₂ -(² D)6s ³ D ₂
9	976.221	102 435.8	.83	(² P)4d ³ P ₂ -(² P)5p ³ P ₁
12 a Sr III	979.166	102 127.7	9.37	(² P)4d ³ P ₂ -(² P)5p ³ S ₁
9	972.142	102 865.6	.55	(² D)4d ³ D ₁ -(⁴ S)5p ³ P ₁
10	969.104	103 188.1	.20	(² P)4d ³ F ₂ -(² P)5p ³ D _{1</}

Table I. Continued

Intensity and shape	$\lambda_{vac.}$ (Å)	σ (cm ⁻¹)		Classification
		Obs.	Calc.	
3	937.441	106 673.3	.72	(² D)4d ³ G ₃ -(² D)5p ³ F ₃
12	936.808	106 745.5	.44	(² D)4d ³ G ₃ -(² D)5p ³ D ₂
12 bl 2 × Sr V	935.506	106 894.0	3.65	(² P)4d ³ F ₃ -(² P)5p ³ D ₂
10	930.619	107 455.3	.23	(² D)4d ³ D ₃ -(⁴ S)5p ³ P ₂
10	928.354	107 717.5	.67	(² D)4d ³ G ₄ -(² D)5p ¹ F ₃
12	927.356	107 833.5	.5	(² D)4d ³ G ₅ -(² D)5p ³ F ₄
8	924.103	108 213.0	.71	(² P)4d ³ P ₂ -(² P)5p ¹ P ₁
12	922.397	108 413.2	.2	(² P)4d ³ F ₄ -(² P)5p ³ D ₃
0.5	921.189	108 555.4	4.95	(² P)4d ³ P ₁ -(² P)5p ³ D ₂
8	916.201	109 146.4	.34	(² P)4d ³ D ₃ -(² P)5p ¹ D ₂
8	915.456	109 235.1	6.02	(² P)4d ³ P ₁ -(² P)5p ³ S ₁
9	913.913	109 419.6	.80	(² D)4d ¹ S ₀ -(² D)5p ³ D ₁
9	911.014	109 767.8	8.02	(² P)4d ³ P ₂ -(² P)5p ³ P ₂
8	910.270	109 857.5	8.00	(² P)4d ¹ D ₂ -(² D)5p ¹ D ₂
7 u	909.308	109 973.7	{ .34 .77	(² D)4d ³ S ₁ -(² P)5p ¹ S ₀ (² P)4d ³ F ₃ -(² P)5p ³ D ₃
6	908.568	110 063.3	.75	(² P)4d ³ P ₁ -(² P)5p ³ P ₀
7	905.416	110 446.5	.47	(² P)4d ³ P ₀ -(² P)5p ³ S ₁
9	903.765	110 648.3	.52	(² D)4d ³ F ₂ -(² D)5p ³ D ₁
0.5	898.766	111 263.7	.64	(² P)4d ³ D ₂ -(² P)5p ³ D ₃
12	897.619	111 405.8	.51	(⁴ S)4d ⁵ D ₂ -(⁴ S)5p ⁵ P ₁
9 a	897.163	111 462.5	1.76	(⁴ S)4d ⁵ D ₁ -(⁴ S)5p ⁵ P ₁
9	896.495	111 545.5	6.12	(² P)4d ³ D ₃ -(² P)5p ³ P ₂
12	896.073	111 598.1	.28	(⁴ S)4d ⁵ D ₀ -(⁴ S)5p ⁵ P ₁
15	894.896	111 744.8	.70	(⁴ S)4d ⁵ D ₃ -(⁴ S)5p ⁵ P ₂
12	894.626	111 778.6	.91	(² D)4d ³ F ₄ -(² D)5p ³ F ₃
15	894.277	111 822.2	1.75	(⁴ S)4d ⁵ D ₂ -(⁴ S)5p ⁵ P ₂
10	893.829	111 878.2	.00	(⁴ S)4d ⁵ D ₁ -(⁴ S)5p ⁵ P ₂
9	889.956	112 365.1	.28	(² P)4d ¹ D ₂ -(² P)5p ³ D ₁
8	887.507	112 675.1	.69	(² P)4d ³ F ₂ -(² P)5p ¹ P ₁
9 u	886.418	112 813.6	.59	(² P)4d ³ F ₃ -(² P)5p ¹ D ₂
15	883.338	113 206.9	.94	(⁴ S)4d ⁵ D ₄ -(⁴ S)5p ⁵ P ₃
3	880.021	113 633.6	.71	(² D)4d ³ G ₃ -(² D)5p ³ P ₂
12	879.343	113 721.3	.42	(⁴ S)4d ⁵ D ₃ -(⁴ S)5p ⁵ P ₃
8	878.746	113 798.5	.47	(⁴ S)4d ⁵ D ₂ -(⁴ S)5p ⁵ P ₃
10	878.621	113 814.7	5.15	(² D)4d ³ F ₂ -(² D)5p ³ F ₂
9 bl 2 × Sr V	878.360	113 848.5	7.48	(² D)4d ³ F ₃ -(² D)5p ¹ F ₃
9	875.432	114 229.4	{ 29.05 30.00	(² D)4d ³ D ₁ -(² D)5p ³ D ₁ (² P)4d ³ F ₂ -(² P)5p ³ P ₂
9	875.239	114 254.4	.93	(² D)4d ³ F ₃ -(² D)5p ³ F ₃
7	873.373	114 498.6	9.13	(² P)4d ³ D ₁ -(² P)5p ³ P ₀
10	868.914	115 086.1	{ 5.82 7.36	(² D)4d ³ F ₄ -(² D)5p ³ D ₃ (² P)4d ¹ D ₂ -(² P)5p ³ D ₂
4	867.161	115 318.9	20.36	(² P)4d ³ P ₁ -(² P)5p ¹ P ₁
10	865.236	115 575.4	.04	(² D)4d ³ F ₄ -(² D)5p ³ F ₄
8	864.484	115 675.9	.86	(² D)4d ¹ S ₀ -(² D)5p ¹ P ₁
9	861.522	116 073.6	{ 3.55 4.89	(² D)4d ³ F ₂ -(² D)5p ³ F ₃ (² P)4d ¹ D ₂ -(² P)5p ³ P ₁
0.5	860.992	116 145.1	.27	(² D)4d ³ F ₂ -(² D)5p ³ D ₂
6	859.670	116 323.7	.50	(² D)4d ³ F ₃ -(² D)5p ¹ F ₃
5	858.345	116 503.3	.24	(² P)4d ³ D ₂ -(² P)5p ³ P ₂
3 a C II	858.130	116 532.4	0.81	(² P)4d ³ P ₀ -(² P)5p ¹ P ₁
5	855.618	116 874.7	.67	(² P)4d ³ P ₁ -(² P)5p ³ P ₂
10	855.398	116 904.6	.58	(² D)4d ³ F ₂ -(² D)5p ¹ P ₁
9 u, bl Sr IV	851.796	117 399.0	5.68	(² D)4d ³ D ₁ -(² D)5p ³ F ₂
5 a	851.681	117 414.9	.42	(² D)4d ³ D ₂ -(² D)5p ³ D ₁
0.5	850.974	117 512.4	3.31	(⁴ S)4d ⁵ D ₂ -(⁴ S)5p ⁵ P ₁
6	850.573	117 567.8	9.56	(⁴ S)4d ⁵ D ₁ -(⁴ S)5p ⁵ P ₁
5	849.572	117 706.3	.08	(⁴ S)4d ⁵ D ₀ -(⁴ S)5p ⁵ P ₁

Table I. Continued

Intensity and shape	$\lambda_{vac.}$ (Å)	σ (cm ⁻¹)		Classification
		Obs.	Calc.	
8	847.090	118 051.1	.06	(² D)4d ³ F ₂ -(² D)5p ³ F ₄
0.5	846.275	118 164.9	7.48	(² P)4d ¹ D ₂ -(² P)5p ³ D ₃
7	845.590	118 260.6	.70	(² D)4d ³ D ₃ -(² D)5p ³ F ₂
8	841.463	118 840.6	.57	(⁴ S)4d ⁵ D ₃ -(⁴ S)5p ³ P ₂
8	840.919	118 917.6	.62	(⁴ S)4d ⁵ D ₂ -(⁴ S)5p ³ P ₂
7	840.517	118 974.4	3.87	(⁴ S)4d ⁵ D ₁ -(⁴ S)5p ³ P ₂
6	829.977	120 485.3	.11	(² D)4d ³ D ₁ -(² D)5p ¹ P ₁
10 u, a Sr IV	829.248	120 591.2	0.82	(² D)4d ³ D ₃ -(² D)5p ³ D ₂
8	826.395	121 007.5	.30	(² P)4d ¹ D ₂ -(² P)5p ¹ D ₂
6	824.979	121 215.3	4.92	(² D)4d ³ F ₃ -(² D)5p ³ P ₂
0.5	823.805	121 387.9	.92	(² D)4d ³ G ₃ -(² D)5p ¹ D ₂
7	820.662	121 852.9	.77	(² P)4d ¹ D ₂ -(² P)5p ¹ P ₁
9	815.745	122 587.3	.67	(² D)4d ³ D ₃ -(² D)5p ¹ F ₃
5	814.070	122 839.6	.45	(² D)4d ³ D ₂ -(² D)5p ³ F ₃
9	813.597	122 910.9	1.17	(² D)4d ³ D ₂ -(² D)5p ³ D ₂
4	812.790	123 033.0	.54	(² D)4d ³ F ₂ -(² D)5p ³ P ₂
8	808.602	123 670.2	.48	(² D)4d ³ D ₂ -(² D)5p ¹ P ₁
8	807.593	123 824.7	6.01	(² D)4d ³ D ₃ -(² D)5p ³ D ₃
6	804.403	124 315.8	.23	(² D)4d ³ D ₃ -(² D)5p ³ F ₄
4	801.313	124 795.2	4.50	(² D)4d ³ F ₂ -(² D)5p ³ P ₁
5	800.591	124 907.7	8.02	(² D)4d ³ D ₂ -(² D)5p ¹ F ₃
7	784.436	127 480.1	79.09	(² D)4d ³ D ₃ -(² D)5p ³ P ₂
4	780.719	128 087.1	8.15	(² D)4d ³ D ₁ -(² D)5p ³ P ₀
2 a	778.982	128 372.7	5.03	(² D)4d ³ D ₁ -(² D)5p ³ P ₁
2	777.164	128 673.0	2.78	(² D)4d ³ G ₄ -(² P)5p ³ D ₃
6	770.425	129 798.5	9.44	(² D)4d ³ D ₂ -(² D)5p ³ P ₂
2 a	760.117	131 558.7	60.40	(² D)4d ³ D ₂ -(² D)5p ³ P ₁
4	757.193	132 066.7	.31	(² D)4d ¹ S ₀ -(² P)5p ³ D ₁
2	693.802	144 133.4	5.43	4s4p ⁵ ¹ P ₁ -(² D)5p ¹ P ₁
3 h	591.127	169 168.5	7.90	4s4p ⁵ ¹ P ₁ -(² P)5p ¹ D ₂
4	584.174	171 181.8	0.72	4s4p ⁵ ³ P ₁ -(² D)5p ³ D ₁
m Sr VI		177 165.	.95	4s4p ⁵ ³ P ₂ -(² D)5p ³ D ₁
3 h	551.491	181 326.5	8.54	4s4p ⁵ ³ P ₀ -(² D)5p ³ P ₁
3	549.960	181 831.3	3.29	4s4p ⁵ ¹ P ₁ -(² P)5p ¹ S ₀
3	547.460	182 661.9	2.70	4s4p ⁵ ³ P ₂ -(² D)5p ³ D ₂
9	546.321	183 042.7	.51	(⁴ S)4d ⁵ D ₄ -(⁴ S)4f ⁵ F ₄
2 h Sr V?	545.590	183 287.9	6.84	(⁴ S)4d ⁵ D ₄ -(⁴ S)4f ⁵ F ₃
12	544.790	183 556.8	.99	(⁴ S)4d ⁵ D ₃ -(⁴ S)4f ⁵ F ₄
12	544.281	183 728.6	.6	(⁴ S)4d ⁵ D ₃ -(⁴ S)4f ⁵ F ₅
10	544.066	183 801.2	.32	(⁴ S)4d ⁵ D ₃ -(⁴ S)4f ⁵ F ₃
10	543.837	183 878.5	.37	(⁴ S)4d ⁵ D ₂ -(⁴ S)4f ⁵ F ₃
4	543.358	184 040.7	1.23	(⁴ S)4d ⁵ D ₃ -(⁴ S)4f ⁵ F ₂
9	543.128	184 118.8	.28	(⁴ S)4d ⁵ D ₂ -(⁴ S)4f ⁵ F ₂
9	542.963	184 174.6	.53	(⁴ S)4d ⁵ D ₁ -(⁴ S)4f ⁵ F ₂
2 Sr V?	542.478	184 339.5	.13	(⁴ S)4d ⁵ D ₂ -(⁴ S)4f ⁵ F ₁
9 a	542.319	184 393.3	5.38	(⁴ S)4d ⁵ D ₁ -(⁴ S)4f ⁵ F ₁
9	541.913	184 531.6	.90	(⁴ S)4d ⁵ D ₀ -(⁴ S)4f ⁵ F ₁
8	527.559	189 552.4	0.97	4s4p ⁵ ³ P ₂ -(² D)5p ³ P ₂
7	522.702	191 313.7	1.93	4s4p ⁵ ³ P ₂ -(² D)5p ³ P ₁
1 a Sr V	392.024	255 086.2	5.94	(⁴ S)4d ⁵ D ₄ -(⁴ S)5f ⁵ F ₄
8	391.236	255 600.2	.42	(⁴ S)4d ⁵ D ₃ -(⁴ S)5f ⁵ F ₄
1	390.753	255 916.2	5.79	(⁴ S)4d ⁵ D ₃ -(⁴ S)5f ⁵ F ₃
8	390.636	255 992.5	.84	(⁴ S)4d ⁵ D ₂ -(⁴ S)5f ⁵ F ₃
9	390.571	256 034.6	.43	(⁴ S)4d ⁵ D ₄ -(⁴ S)5f ⁵ F ₅
0.5	390.209	256 273.1	5.48	(⁴ S)4d ⁵ D ₂ -(⁴ S)5f ⁵ F ₂
5	390.119	256 332.2	1.73	(⁴ S)4d ⁵ D ₁ -(⁴ S)5f ⁵ F ₂
6	389.515	256 729.8	.8	(⁴ S)4d ⁵ D ₀ -(⁴ S)5f ⁵ F ₁

Table II. Observed resonance lines of Sr V. Abbreviation for line characteristic: bl = blended (by). Intensities are uncorrected visual estimates of the photographic densities of the lines. All levels are given in LS notation

Intensity and shape	$\lambda_{\text{Obs.}} (\text{\AA})$	$\sigma (\text{cm}^{-1})$		Classification	$\lambda_{\text{Calc.}} (\text{\AA})$
		Obs.	Calc.		
9	862.316	115 966.7	7.11	$4s^2 4p^4 \ ^1S_0 - 4s 4p^5 \ ^3P_1$	862.3135
12	747.823	133 721.5	1.78	$\ ^1D_2 - \ ^3P_2$	747.8213
6	715.787	139 706.3	7.01	$\ ^1D_2 - \ ^3P_1$	715.7837
35	686.228	145 724.2	4.41	$\ ^3P_1 - \ ^3P_2$	686.2268
9	669.933	149 268.6	8.46	$\ ^1S_0 - \ ^1P_1$	669.9339
25	660.943	151 299.1	9.05	$\ ^3P_0 - \ ^3P_1$	660.9427
20	659.153	151 710.0	9.64	$\ ^3P_1 - \ ^3P_1$	659.1539
50	649.213	154 032.8	2.29	$\ ^3P_2 - \ ^3P_2$	649.2145
25	642.229	155 707.8	7.80	$\ ^3P_1 - \ ^3P_0$	642.2286
30	624.932	160 017.5	7.52	$\ ^3P_2 - \ ^3P_1$	624.9316
25	578.006	173 008.6	8.36	$\ ^1D_2 - \ ^1P_1$	578.0068
6	540.509	185 010.7	0.99	$\ ^3P_1 - \ ^1P_1$	540.5084
10	517.281	193 318.4	8.87	$\ ^3P_2 - \ ^1P_1$	517.2801
7	516.672	193 546.5	6.71	$\ ^3P_0 - (^4S)4d \ ^5D_1$	516.6711
9	515.938	193 821.9	0.78	$\ ^3P_1 - (^4S)4d \ ^5D_0$	515.9406
9	515.578	193 957.2	7.30	$\ ^3P_1 - (^4S)4d \ ^5D_1$	515.5774
8	494.916	202 054.6	7.83	$\ ^1D_2 - (^2D)4d \ ^3F_3$	494.9078
12	494.391	202 268.9	5.18	$\ ^3P_2 - (^4S)4d \ ^5D_1$	494.4005
18	494.263	202 321.5	1.43	$\ ^3P_2 - (^4S)4d \ ^5D_2$	494.2630
15	494.075	202 398.5	8.48	$\ ^3P_2 - (^4S)4d \ ^5D_3$	494.0749
8	486.678	205 474.7	5.94	$\ ^3P_1 - (^2D)4d \ ^3D_2$	486.6750
10	480.193	208 249.7	50.72	$\ ^3P_0 - (^2D)4d \ ^3D_1$	480.1904
12	479.244	208 661.9	1.31	$\ ^3P_1 - (^2D)4d \ ^3D_1$	479.2455
15	477.014	209 637.6	9.04	$\ ^1D_2 - (^2D)4d \ ^3G_3$	477.0104
7	471.164	212 240.1	1.84	$\ ^3P_1 - (^2D)4d \ ^3F_2$	471.1606
4	468.447	213 471.5	0.56	$\ ^3P_1 - (^2D)4d \ ^1S_0$	468.4487
20	467.761	213 784.6	3.82	$\ ^3P_2 - (^2D)4d \ ^3D_2$	467.7622
18	462.739	216 104.6	4.17	$\ ^3P_2 - (^2D)4d \ ^3D_3$	462.7398
9	460.908	216 963.0	9.19	$\ ^3P_2 - (^2D)4d \ ^3D_1$	460.8949
15	453.414	220 549.2	9.72	$\ ^3P_2 - (^2D)4d \ ^3F_2$	453.4125
20	452.142	221 169.6	8.96	$\ ^1D_2 - (^2P)4d \ ^1D_2$	452.1430
18	449.706	222 367.5	8.34	$\ ^3P_2 - (^2D)4d \ ^3F_3$	449.7043
10	447.897	223 265.9	5.99	$\ ^1D_2 - (^2P)4d \ ^3D_1$	447.8963
7	443.332	225 564.5	4.41	$\ ^1S_0 - (^2D)4d \ ^3P_1$	443.3324
15	439.170	227 702.5	1.37	$\ ^1D_2 - (^2P)4d \ ^3P_1$	439.1717
0.5	438.456	228 073.3	2.80	$\ ^1D_2 - (^2P)4d \ ^3D_2$	438.4565
18	435.990	229 363.1	2.67	$\ ^1D_2 - (^2P)4d \ ^3F_3$	435.9907
18	434.878	229 949.4	9.55	$\ ^3P_2 - (^2D)4d \ ^3G_3$	434.8780
18	434.129	230 346.4	6.04	$\ ^1D_2 - (^2P)4d \ ^3F_2$	434.1295
8	433.084	230 902.0	1.33	$\ ^1S_0 - (^4S)5s \ ^3S_1$	433.0854
10	432.081	231 438.3	7.72	$\ ^1S_0 - (^2D)4d \ ^1P_1$	432.0817
18	429.128	233 030.5	29.92	$\ ^1D_2 - (^2P)4d \ ^3D_3$	429.1294
9	428.867	233 172.6	1.59	$\ ^3P_1 - (^2P)4d \ ^1D_2$	428.8687
7	425.878	234 809.3	8.02	$\ ^1D_2 - (^2P)4d \ ^3P_2$	425.8798
25	425.790	234 857.4	8.03	$\ ^3P_0 - (^2P)4d \ ^3D_1$	425.7891
15	425.042	235 270.8	68.62	$\ ^3P_1 - (^2P)4d \ ^3D_1$	425.0461
9	419.296	238 494.9	3.55	$\ ^3P_1 - (^2P)4d \ ^3P_0$	419.2986
8	417.896	239 294.3	3.41	$\ ^3P_0 - (^2P)4d \ ^3P_1$	417.8970
18	417.180	239 704.5	4.00	$\ ^3P_1 - (^2P)4d \ ^3P_1$	417.1812
30	416.532	240 077.4	5.43	$\ ^3P_1 - (^2P)4d \ ^3D_2$	416.5358
15	414.112	241 480.9	79.47	$\ ^3P_2 - (^2P)4d \ ^1D_2$	414.1139
25	412.627	242 349.7	8.67	$\ ^3P_1 - (^2P)4d \ ^3F_2$	412.6286
6	410.551	243 575.0	6.50	$\ ^3P_2 - (^2P)4d \ ^3D_1$	410.5486
12	408.384	244 867.6	8.31	$\ ^1D_2 - (^2D)4d \ ^3S_1$	408.3828
15	406.622	245 929.0	8.91	$\ ^1D_2 - (^2P)4d \ ^1F_3$	406.6216
8	406.480	246 014.7	4.82	$\ ^1D_2 - (^4S)5s \ ^5S_2$	406.4796
18	405.168	246 811.1	0.65	$\ ^3P_1 - (^2P)4d \ ^3P_2$	405.1689
15	404.796	247 038.2	40.52	$\ ^1D_2 - (^2D)4d \ ^3P_2$	404.7919
20	403.204	248 013.4	1.88	$\ ^3P_2 - (^2P)4d \ ^3P_1$	403.2065
5	402.597	248 387.2	3.31	$\ ^3P_2 - (^2P)4d \ ^3D_2$	402.6035
20	401.117	249 303.7	4.31	$\ ^1D_2 - (^2D)4d \ ^3P_1$	401.1162
20	400.523	249 673.8	3.18	$\ ^3P_2 - (^2P)4d \ ^3F_3$	400.5236
1	398.102	251 192.0	89.68	$\ ^1D_2 - (^4S)4d \ ^3D_3$	398.1055
40	394.724	253 341.6	0.43	$\ ^3P_2 - (^2P)4d \ ^3D_3$	394.7258
20	392.709	254 641.2	1.23	$\ ^1D_2 - (^4S)5s \ ^3S_1$	392.7094
25	391.975	255 118.6	8.53	$\ ^3P_2 - (^2P)4d \ ^3P_2$	391.9747
20	391.884	255 177.5	7.62	$\ ^1D_2 - (^2D)4d \ ^1P_1$	391.8839

Table II. Continued

Intensity and shape	$\lambda_{\text{Obs.}} (\text{\AA})$	$\sigma (\text{cm}^{-1})$		Classification	$\lambda_{\text{Calc.}} (\text{\AA})$
		Obs.	Calc.		
10	389.920	256 462.9	0.35	$^3P_0 - (^2D)4d \ ^3S_1$	389.9238
18	389.848	256 510.1	0.95	$^1D_2 - (^4S)4d \ ^3D_2$	389.8469
18	389.298	256 872.7	0.94	$^3P_1 - (^2D)4d \ ^3S_1$	389.3006
18	387.569	258 018.4	7.45	$^3P_1 - (^4S)5s \ ^5S_2$	387.5707
20	386.034	259 044.9	3.15	$^3P_1 - (^2D)4d \ ^3P_2$	386.0361
15	384.975	259 757.4	6.58	$^1D_2 - (^4S)4d \ ^3D_1$	384.9758
18	383.294	260 896.2	6.35	$^3P_0 - (^2D)4d \ ^3P_1$	383.2940
20	382.690	261 308.2	6.94	$^3P_1 - (^2D)4d \ ^3P_1$	382.6917
20	381.642	262 025.5	4.99	$^1S_0 - (^2P)4d \ ^1P_1$	381.6430
18	379.137	263 757.1	6.04	$^1S_0 - (^2P)5s \ ^3P_1$	379.1382
30	377.162	265 138.3	9.53	$^1D_2 - (^2D)4d \ ^1D_2$	377.1599
30	377.106	265 177.2	8.82	$^3P_2 - (^2D)4d \ ^3S_1$	377.1040
18	375.602	266 239.1	3.27	$^3P_0 - (^4S)5s \ ^3S_1$	375.6105
			9.42	$^3P_2 - (^2P)4d \ ^1F_3$	375.6018
35	375.480	266 325.7	5.33	$^3P_2 - (^4S)5s \ ^5S_2$	375.4806
18	375.033	266 643.1	3.86	$^3P_1 - (^4S)5s \ ^3S_1$	375.0321
20	374.861	266 765.8	9.66	$^3P_0 - (^2D)4d \ ^1P_1$	374.8552
20	374.366	267 118.2	7.53	$^3P_1 - (^2D)4d \ ^3P_0$	374.3670
20	374.280	267 179.4	80.25	$^3P_1 - (^2D)4d \ ^1P_1$	374.2792
50	374.043	267 348.7	51.03	$^3P_2 - (^2D)4d \ ^3P_2$	374.0401
35	372.423	268 512.1	3.58	$^3P_1 - (^4S)4d \ ^3D_2$	372.4206
18	372.018	268 804.1	6.15	$^1D_2 - (^2D)5s \ ^3D_2$	372.0153
20	370.906	269 610.2	4.82	$^3P_2 - (^2D)4d \ ^3P_1$	370.8995
18	369.430	270 687.2	5.53	$^1S_0 - (^2P)5s \ ^1P_1$	369.4324
20	368.532	271 346.6	8.62	$^3P_0 - (^4S)4d \ ^3D_1$	368.5296
15	368.507	271 365.4	7.90	$^1D_2 - (^2D)4d \ ^1F_3$	368.5034
50	368.326	271 498.8	500.19	$^3P_2 - (^4S)4d \ ^3D_3$	368.3239
35	368.295	271 521.7	5.06	$^1D_2 - (^2D)5s \ ^3D_3$	368.2901
25	367.976	271 757.2	9.21	$^3P_1 - (^4S)4d \ ^3D_1$	367.9728
25	364.289	274 507.4	7.64	$^1D_2 - (^2D)5s \ ^1D_2$	364.2886
20	363.700	274 952.2	1.74	$^3P_2 - (^4S)5s \ ^3S_1$	363.7002
25	361.245	276 820.7	1.46	$^3P_2 - (^4S)4d \ ^3D_2$	361.2437
20	360.824	277 143.6	2.16	$^3P_1 - (^2D)4d \ ^1D_2$	360.8256
9	357.055	280 068.8	7.09	$^3P_2 - (^4S)4d \ ^3D_1$	357.0573
12	356.999	280 113.1	3.15	$^3P_0 - (^2D)5s \ ^3D_1$	356.9986
20	356.475	280 524.7	3.74	$^3P_1 - (^2D)5s \ ^3D_1$	356.4761
20	356.113	280 810.0	08.78	$^3P_1 - (^2D)5s \ ^3D_2$	356.1142
9	350.323	285 450.8	0.04	$^3P_2 - (^2D)4d \ ^1D_2$	350.3240
7	349.935	285 767.4	4.89	$^1D_2 - (^2P)4d \ ^1P_1$	349.9380
10	349.027	286 510.7	0.27	$^3P_1 - (^2D)5s \ ^1D_2$	349.0276
9	347.831	287 496.0	5.94	$^1D_2 - (^2P)5s \ ^3P_1$	347.8310
25	345.882	289 116.1	6.66	$^3P_2 - (^2D)5s \ ^3D_2$	345.8811
18	343.184	291 389.0	9.24	$^1D_2 - (^2P)5s \ ^3P_2$	343.1836
40	342.848	291 674.8	8.41	$^3P_2 - (^2D)4d \ ^1F_3$	342.8433
0.5	342.654	291 839.4	5.57	$^3P_2 - (^2D)5s \ ^3D_3$	342.6587
12	339.644	294 425.6	5.43	$^1D_2 - (^2P)5s \ ^1P_1$	339.6446
10	339.195	294 815.8	8.15	$^3P_2 - (^2D)5s \ ^1D_2$	339.1921
3	336.295	297 357.9	6.93	$^3P_0 - (^2P)4d \ ^1P_1$	336.2962
10	335.234	298 299.3	9.52	$^3P_1 - (^2P)5s \ ^3P_0$	335.2335
10	334.351	299 086.7	7.98	$^3P_0 - (^2P)5s \ ^3P_1$	334.3498
9	333.890	299 499.5	8.57	$^3P_1 - (^2P)5s \ ^3P_1$	333.8914
25	329.605	303 393.4	1.87	$^3P_1 - (^2P)5s \ ^3P_2$	329.6067
0.5	326.778	306 017.8	7.47	$^3P_0 - (^2P)5s \ ^1P_1$	326.7787
0.5	326.717	306 075.5	5.40	$^3P_2 - (^2P)4d \ ^1P_1$	326.7169
0.5	326.340	306 428.8	8.06	$^3P_1 - (^2P)5s \ ^1P_1$	326.3409
7	324.878	307 808.0	6.45	$^3P_2 - (^2P)5s \ ^3P_1$	324.8795
10	320.823	311 698.7	9.75	$^3P_2 - (^2P)5s \ ^3P_2$	320.8216
2	274.320	364 537.4	5.67	$^1S_0 - (^2D)5d \ ^3D_1$	274.3216
1	269.203	371 467.0	2.31	$^1D_2 - (^4S)5d \ ^3D_2$	269.2063
6	268.423	372 546.9	5.98	$^1D_2 - (^4S)5d \ ^3D_3$	268.4232
10	260.781	383 463.5	4.94	$^3P_1 - (^4S)5d \ ^3D_2$	260.7800
9	260.426	383 986.2	9.34	$^3P_0 - (^4S)5d \ ^3D_1$	260.4239
8	260.145	384 400.6	399.93	$^3P_1 - (^4S)5d \ ^3D_1$	260.1457
1	260.032	384 568.2	7.79	$^1D_2 - (^4S)6s \ ^3S_1$	260.0322
0.5	258.676	386 583.7	1.90	$^3P_2 - (^4S)5d \ ^5D_2$	258.6774
7	258.416	386 972.6	1.91	$^1D_2 - (^2D)5d \ ^3G_3$	258.4167
			4.00	$^1S_0 - (^2P)5d \ ^3P_1$	258.4153
5	257.951	387 670.8	69.16	$^1D_2 - (^2D)5d \ ^3F_3$	257.9519

Table II. Continued

Intensity and shape	$\lambda_{\text{Obs.}} (\text{\AA})$	$\sigma (\text{cm}^{-1})$		Classification	$\lambda_{\text{Calc.}} (\text{\AA})$
		Obs.	Calc.		
12 bl Sr IV	257.546	388 279.6	5.57	$^1D_2 - (^2D)5d \ ^3D_1$	257.5490
3	256.273	390 208.7	6.36	$^1D_2 - (^2D)5d \ ^3D_2$	256.2747
0.5	255.429	391 498.7	89.63	$^1D_2 - (^2D)5d \ ^3D_3$	255.4346
9	255.249	391 774.0	2.82	$^3P_2 - (^4S)5d \ ^3D_2$	255.2500
8	254.987	392 177.2	5.85	$^1D_2 - (^2D)5d \ ^1P_1$	254.9877
5	254.642	392 707.6	7.81	$^3P_2 - (^4S)5d \ ^3D_1$	254.6422
15	254.545	392 858.6	6.49	$^3P_2 - (^4S)5d \ ^3D_3$	254.5459
6	254.363	393 138.5	5.75	$^1D_2 - (^2D)5d \ ^3P_1$	254.3651
8	253.506	394 467.7	4.58	$^1D_2 - (^2D)5d \ ^3S_1$	253.5082
9	253.379	394 665.7	2.17	$^1S_0 - (^2P)5d \ ^1P_1$	253.3813
10	253.015	395 233.6	1.82	$^1D_2 - (^2D)5d \ ^1D_2$	253.0161
8	252.422	396 161.8	59.83	$^3P_0 - (^4S)6s \ ^3S_1$	252.4234
10	252.160	396 573.8	0.42	$^3P_1 - (^4S)6s \ ^3S_1$	252.1620
12	251.668	397 348.9	7.31	$^1D_2 - (^2D)5d \ ^1F_3$	251.6690
1	251.536	397 557.1	5.9	$^1S_0 - (^2P)6s \ ^3P_1$	251.537
7	251.367	397 824.1	1.23	$^3P_1 - (^2D)5d \ ^3F_2$	251.3692
8	250.084	399 866.0	7.61	$^3P_0 - (^2D)5d \ ^3D_1$	250.0828
12	248.628	402 207.1	8.99	$^3P_1 - (^2D)5d \ ^3D_2$	248.6270
7	248.536	402 355.6	6.59	$^3P_2 - (^4S)6s \ ^5S_2$	248.5358
5	248.265	402 795.2	7.02	$^1D_2 - (^2D)6s \ ^3D_1$	248.2640
9	248.142	402 995.6	2.8	$^1S_0 - (^2P)6s \ ^1P_1$	248.143
8	248.134	403 007.9	5.28	$^1D_2 - (^2D)6s \ ^3D_2$	248.1357
8	247.669	403 765.1	7.89	$^3P_0 - (^2D)5d \ ^1P_1$	247.6670
2	247.417	404 175.8	8.48	$^3P_1 - (^2D)5d \ ^1P_1$	247.4154
2	247.097	404 699.5	9.87	$^3P_1 - (^2D)5d \ ^3P_2$	247.0967
3	247.082	404 724.8	7.79	$^3P_0 - (^2D)5d \ ^3P_1$	247.0796
12	246.989	404 875.7	8.30	$^3P_2 - (^4S)6s \ ^3S_1$	246.9878
9	246.830	405 137.1	8.38	$^3P_1 - (^2D)5d \ ^3P_1$	246.8292
8	246.601	405 512.9	4.54	$^3P_1 - (^2D)5d \ ^3P_0$	246.6003
7	246.303	406 003.8	6.77	$^1D_2 - (^2D)6s \ ^3D_3$	246.3013
1	246.273	406 053.8	6.62	$^3P_0 - (^2D)5d \ ^3S_1$	246.2711
7	246.228	406 127.2	9.11	$^3P_2 - (^2D)5d \ ^3F_2$	246.2271
15	245.760	406 901.5	896.74 906.55	$^1D_2 - (^2P)5d \ ^3D_2$	245.7626
6	245.560	407 232.0	4.45	$^1D_2 - (^2D)6s \ ^1D_2$	245.7567
9	245.533	407 277.2	82.42	$^3P_1 - (^2D)5d \ ^1D_2$	245.5588
2	245.113	407 974.6	9.67	$^3P_2 - (^2D)5d \ ^3G_3$	245.5299
6	244.750	408 580.4	6.08	$^3P_2 - (^2D)5d \ ^3F_3$	245.1103
8	243.599	410 510.1	6.87	$^3P_2 - (^2D)5d \ ^3D_1$	244.7465
2	243.482	410 707.3	13.90	$^3P_2 - (^2D)5d \ ^3D_2$	243.5953
12	242.840	411 793.1	800.14	$^1D_2 - (^2P)5d \ ^3P_1$	243.4785
7	242.437	412 478.6	86.36	$^3P_2 - (^2D)5d \ ^3D_3$	242.8362
9	242.195	412 891.1	2.31	$^3P_2 - (^2D)5d \ ^1P_1$	242.4323
10	242.127	413 006.6	7.75	$^1D_2 - (^2P)5d \ ^3D_3$	242.1939
7	241.926	413 349.7	9.84	$^3P_2 - (^2D)5d \ ^3P_2$	242.1262
6	241.872	413 442.5	6.26	$^1D_2 - (^2P)5d \ ^1F_3$	241.9258
8	241.753	413 645.7	7.68	$^3P_2 - (^2D)5d \ ^3P_1$	241.8694
7	241.321	414 386.2	9.06	$^1D_2 - (^2P)5d \ ^1D_2$	241.7516
8	241.095	414 773.9	5.09	$^3P_0 - (^2D)6s \ ^3D_1$	241.3191
7	241.082	414 797.1	9.65	$^3P_2 - (^2D)5d \ ^3S_1$	241.0945
7	240.959	415 007.7	7.91	$^3P_1 - (^2D)6s \ ^3D_1$	241.0802
8	239.430	417 659.1	7.82	$^3P_1 - (^2D)6s \ ^3D_2$	240.9593
1	239.007	418 398.7	402.07	$^3P_2 - (^2D)5d \ ^1F_3$	239.4305
9	238.720	418 900.5	899.37	$^1D_2 - (^2P)5d \ ^1P_1$	239.0046
8	238.244	419 737.0	7.45	$^3P_1 - (^2P)5d \ ^3D_2$	238.7208
3	238.011	420 148.3	8.04	$^3P_0 - (^2P)5d \ ^3D_1$	238.2442
6	237.364	421 294.4	5.8	$^3P_1 - (^2P)5d \ ^3D_1$	238.0113
6	237.139	421 693.8	3.8	$^1D_2 - (^2P)6s \ ^3P_1$	237.363
8	236.566	422 715.4	6.53	$^3P_1 - (^2P)5d \ ^3P_0$	237.139
9	236.231	423 314.6	5.79	$^3P_1 - (^2P)5d \ ^3P_1$	236.5652
3	236.189	423 391.4	2.61	$^3P_2 - (^2D)6s \ ^3D_2$	236.2303
8	234.935	425 650.4	0.31	$^3P_1 - (^2P)5d \ ^3P_2$	236.1874
7	234.768	425 952.4	2.4	$^3P_1 - (^2P)5d \ ^1D_2$	234.9346
10	234.568	426 314.9	7.28	$^1D_2 - (^2P)6s \ ^3P_2$	234.768
8	234.340	426 729.9	32.7	$^3P_2 - (^2D)6s \ ^3D_3$	234.5671
2	234.074	427 214.8	7.06	$^1D_2 - (^2P)6s \ ^1P_1$	234.339
0.5	232.341	430 401.5	4.70	$^3P_2 - (^2D)6s \ ^1D_2$	234.0730
2	231.644	431 697.1	700.49	$^3P_1 - (^2P)5d \ ^1P_1$	232.3395
				$^3P_2 - (^2P)5d \ ^3P_2$	231.6421

Table II. *Continued*

Intensity and shape	$\lambda_{\text{Obs.}} (\text{\AA})$	$\sigma (\text{cm}^{-1})$		Classification	$\lambda_{\text{Calc.}} (\text{\AA})$
		Obs.	Calc.		
9	231.005	432 890.3	87.8	$^3P_0 - (^2P)6s \ ^3P_1$	231.007
4	230.839	433 201.4	2.82	$^3P_2 - (^2P)5d \ ^3D_3$	230.8388
3	230.789	433 296.0	8.4	$^3P_1 - (^2P)6s \ ^3P_1$	230.788
5	230.596	433 659.8	60.35	$^3P_2 - (^2P)5d \ ^1F_3$	230.5952
0.5	230.438	433 955.6	8.19	$^3P_2 - (^2P)5d \ ^1D_2$	230.4369
8	228.333	437 955.9	5.0	$^3P_1 - (^2P)6s \ ^3P_2$	228.334
2	226.446	441 606.4	6.3	$^3P_2 - (^2P)6s \ ^3P_1$	226.446
6	224.084	446 262.0	2.9	$^3P_2 - (^2P)6s \ ^3P_2$	224.083

Table III. *Even levels of Sr V. All levels are given in LS notation. The numbers in parentheses indicate the purities (in %) of the states. Level values given to only one decimal have been determined from one line only*

Designation	$E (\text{cm}^{-1})$
$4s^2 4p^4 \ ^3P_2$	0.00 (94)
$\ ^3P_1$	8 307.88 (100)
$\ ^3P_0$	8 718.47 (91)
$\ ^1D_2$	20 310.51 (94)
$\ ^1S_0$	44 050.41 (91)
$4s^2 4p^3 (^4S) 5p \ ^5P_3$	316 119.90 (95)
$\ ^5P_2$	314 143.18 (84)
$\ ^5P_1$	313 726.94 (91)
$\ ^3P_2$	321 239.05 (78)
$\ ^3P_1$	319 834.74 (73)
$\ ^3P_0$	321 640.81 (90)
$(^2D) 5p \ ^3F_4$	340 419.40 (100)
$\ ^3F_3$	336 623.27 (67)
$\ ^3F_2$	334 364.87 (48)
$\ ^3D_3$	339 930.18 (46)
$\ ^3D_2$	336 694.99 (51)
$\ ^3D_1$	331 198.24 (40)
$\ ^3P_2$	343 583.26 (69)
$\ ^3P_1$	345 344.22 (68)
$\ ^3P_0$	345 057.34 (88)
$\ ^1F_3$	338 691.84 (60)
$\ ^1D_2$	351 337.47 (73)
$\ ^1P_1$	337 454.30 (46)
$(^2P) 5p \ ^3D_3$	359 646.95 (81)
$\ ^3D_2$	356 566.83 (75)
$\ ^3D_1$	353 844.75 (73)
$\ ^3P_2$	364 886.55 (63)
$\ ^3P_1$	357 554.36 (65)
$\ ^3P_0$	358 075.63 (91)
$\ ^3S_1$	357 247.90 (74)
$\ ^1D_2$	362 486.77 (74)
$\ ^1P_1$	363 332.24 (40)
$\ ^1S_0$	375 152.16 (87)
$4s^2 4p^3 (^4S) 4f \ ^5F_5$	386 641.6
$\ ^5F_4$	385 955.47
$\ ^5F_3$	386 199.80
$\ ^5F_2$	386 439.71
$\ ^5F_1$	386 660.56
$4s^2 4p^3 (^4S) 5f \ ^5F_5$	458 947.39
$\ ^5F_4$	457 998.90
$\ ^5F_3$	458 314.27
$\ ^5F_2$	458 596.91
$\ ^5F_1$	458 858.4

Table IV. *Odd levels of Sr V. All levels are given in LS notation. The numbers in parentheses indicate the purities (in %) of the states. Level values given to only one decimal have been determined from only one line or from resonance lines only*

Designation	E (cm ⁻¹)	
$4s4p\ ^5P_2$	154 032.29 (84)	
$\ ^3P_1$	160 017.52 (82)	
$\ ^3P_0$	164 015.68 (84)	
$\ ^1P_1$	193 318.87 (58)	
	$n = 5$	$n = 6$
$4s^24p\ ^3(^4S)ns\ ^5S_2$	266 325.33 (70)	402 356.59 (95)
$\ ^3S_1$	274 951.74 (84)	404 878.30 (93)
$(^2D)ns\ ^3D_3$	291 835.57 (57)	426 317.28 (95)
$\ ^3D_2$	289 116.66 (73)	423 315.79 (63)
$\ ^3D_1$	288 831.62 (84)	423 107.53 (84)
$\ ^1D_2$	294 818.15 (81)	427 217.06 (69)
$(^2P)ns\ ^3P_2$	311 699.75 (78)	446 262.9 (81)
$\ ^3P_1$	307 806.45 (66)	441 606.3 (74)
$\ ^3P_0$	306 607.40 (98)	
$\ ^1P_1$	314 735.94 (76)	447 043.2 (63)
	$n = 4$	$n = 5$
$4s^24p\ ^3(^4S)nd\ ^5D_4$	202 912.96 (96)	386 847.17 (95)
$\ ^5D_3$	202 398.48 (94)	386 627.19 (92)
$\ ^5D_2$	202 321.43 (96)	386 581.90 (93)
$\ ^5D_1$	202 265.18 (97)	386 568.48 (95)
$\ ^5D_0$	202 128.66 (97)	386 524.69 (95)
$\ ^3D_3$	271 500.19 (38)	392 856.49 (87)
$\ ^3D_2$	276 821.46 (30)	391 772.82 (81)
$\ ^3D_1$	280 067.09 (31)	392 707.81 (89)
$(^2D)nd\ ^3G_5$	232 585.9 (100)	411 192.9 (100)
$\ ^3G_4$	230 974.17 (76)	408 237.78 (54)
$\ ^3G_3$	229 949.55 (86)	407 282.42 (60)

Table IV. *Continued*

Designation	E (cm ⁻¹)	
$\ ^3F_4$	224 844.36 (72)	410 365.34 (66)
$\ ^3F_3$	222 368.34 (67)	407 979.67 (54)
$\ ^3F_2$	220 549.72 (57)	406 129.11 (75)
$\ ^3D_3$	216 104.17 (40)	411 800.14 (78)
$\ ^3D_2$	213 783.82 (29)	410 516.87 (42)
$\ ^3D_1$	216 969.19 (47)	408 586.08 (49)
$\ ^3P_2$	267 351.03 (56)	413 007.75 (37)
$\ ^3P_1$	269 614.82 (33)	413 446.26 (37)
$\ ^3P_0$	275 425.41 (58)	413 822.42 (85)
$\ ^3S_1$	265 178.82 (88)	414 775.09 (46)
$\ ^1G_4$	234 782.57 (86)	411 152.84 (40)
$\ ^1F_3$	291 678.41 (32)	417 657.82 (80)
$\ ^1D_2$	285 450.04 (59)	415 542.33 (66)
$\ ^1P_1$	275 488.13 (35)	412 486.36 (29)
$\ ^1S_0$	221 778.44 (95)	
$(^2P)nd\ ^3F_4$	251 233.8 (74)	
$\ ^3F_3$	249 673.18 (76)	
$\ ^3F_2$	250 656.55 (63)	
$\ ^3D_3$	253 340.43 (38)	433 202.82 (41)
$\ ^3D_2$	248 383.31 (49)	427 207.25 (41)
$\ ^3D_1$	243 576.50 (50)	428 455.92 (60)
$\ ^3P_2$	255 118.53 (80)	431 700.49 (50)
$\ ^3P_1$	248 011.88 (70)	431 024.41 (58)
$\ ^3P_0$	246 801.43 (66)	430 001.7 (84)
$\ ^1F_3$	266 239.42 (54)	433 660.35 (39)
$\ ^1D_2$	241 479.47 (58)	433 958.19 (28)
$\ ^1P_1$	306 075.40 (66)	438 712.58 (74)

Table V. *Calculated Sr III, Sr IV and Sr V wavelengths in the 900–200 Å range*

Observed intensity	Calculated wavelength (Å)	Ion	Observed intensity	Calculated wavelength (Å)	Ion	Observed intensity	Calculated wavelength (Å)	Ion	Observed intensity	Calculated wavelength (Å)	Ion
9	862.3135	V	20	501.2955	IV	15	449.4736	IV	9	419.2986	V
12	747.8213	V	18	498.6804	IV	10	447.8963	V	8	417.8970	V
6	715.7837	V	25	491.782	III	7	443.3324	V	18	417.1812	V
35	686.2268	V	8	494.9078	V	25	442.7302	IV	30	416.5358	V
9	669.9339	V	12	494.4005	V	15	440.1472	IV	40	415.3243	IV
25	660.9427	V	18	494.2630	V	15	439.1717	V	15	414.1139	V
20	659.1539	V	15	494.0749	V	0.5	438.4565	V	40	413.0647	IV
50	649.2145	V	20	488.4160	IV	20	437.6558	IV	30	412.9304	IV
25	642.2286	V	20	488.2599	IV	20	437.3417	IV	25	412.6286	V
30	624.9316	V	8	486.6750	V	18	437.237	III	12	412.1026	IV
25	578.0068	V	25	484.2049	IV	18	435.9907	V	20	410.6711	IV
20	562.752	III	10	480.1904	V	18	434.8780	V	6	410.5486	V
6	560.8645	IV	12	479.2455	V	18	434.1295	V	12	408.3828	V
6	540.5084	V	20	478.6113	IV	8	433.0854	V	35	406.9426	IV
25	534.1859	IV	15	477.0104	V	10	432.0817	V	15	406.6216	V
18	531.8467	IV	25	471.7580	IV	30	430.6439	IV	8	406.4796	V
10	517.2801	V	7	471.1606	V	20	430.3576	IV	18	405.1689	V
7	516.6711	V	4	468.4487	V	25	430.2118	IV	15	404.7919	V
9	515.9406	V	20	467.7622	V	18	429.1294	V	35	403.8494	IV
9	515.5774	V	20	465.2331	IV	9	428.8687	V	20	403.2065	V
25	514.373	III	18	462.7398	V	7	425.8798	V	5	402.6035	V
15	514.2663	IV	9	460.8949	V	25	425.7891	V	20	401.1162	V
15	512.7796	IV	15	453.4125	V	15	425.0461	V	20	400.5236	V
25	508.1399	IV	20	452.1430	V	15	422.0751	IV	40	399.9252	IV
20	507.033	III	18	449.7043	V	30	419.7836	IV	10	399.1958	IV

Table V. *Continued*

Observed intensity	Calculated wavelength (Å)	Ion	Observed intensity	Calculated wavelength (Å)	Ion	Observed intensity	Calculated wavelength (Å)	Ion	Observed intensity	Calculated wavelength (Å)	Ion
1	398.1055	V	40	342.8433	V	7	270.8654	IV	8	250.2990	IV
50	396.2185	IV	0.5	342.6587	V	6	270.3048	IV	8	250.0828	V
45	394.8951	IV	12	339.6446	V	1	269.2063	V	12	248.6270	V
40	394.7258	V	10	339.1921	V	6	268.4232	V	7	248.5358	V
50	392.9989	IV	3	336.2962	V	8	267.8618	IV	5	248.2640	V
20	392.7094	V	10	335.2335	V	3	266.6899	IV	9	248.143	V
75	392.4324	IV	10	334.3498	V	4	266.3611	IV	8	248.1357	V
25	391.9747	V	5	334.1088	III	1	266.1260	IV	8	247.6670	V
20	391.8839	V	9	333.8914	V	9	264.8352	IV	2	247.4154	V
10	389.9238	V	6	330.6636	III	2	264.6695	IV	2	247.0967	V
18	389.8469	V	25	329.6067	V	7	264.3950	IV	3	247.0796	V
18	389.3006	V	0.5	326.7787	V	6	264.2188	IV	12	246.9878	V
4	388.5834	IV	0.5	326.7169	V	7	264.1616	IV	9	246.8292	V
18	387.5707	V	0.5	326.3409	V	10	263.9270	IV	8	246.6003	V
20	386.0361	V	7	324.8795	V	9	263.9115	IV	7	246.3013	V
15	384.9758	V	5	321.6105	III	7	263.8056	IV	1	246.2711	V
18	383.2940	V	10	320.8216	V	9	263.3792	IV	7	246.2271	V
20	382.6917	V	2	314.3291	IV	10	260.7800	V	15	245.7626	V
20	381.6430	V	5	313.4738	IV	9	260.4239	V	15	245.7567	V
18	379.1382	V	4	310.7067	IV	8	260.1457	V	6	245.5588	V
20	378.5275	IV	9	309.3077	IV	1	260.0322	V	9	245.5299	V
5	377.4154	IV	6	307.0226	IV	2	259.9460	IV	2	245.1103	V
30	377.1599	V	6	306.1795	IV	4	259.6336	IV	6	244.7465	V
30	377.1040	V	5	305.5119	IV	4	259.6112	IV	8	243.5953	V
18	375.6105	V	0.5	305.0028	IV	6	259.4103	IV	2	243.4785	V
35	375.6018	V	10	304.6589	IV	3	259.2386	IV	12	242.8362	V
18	375.4806	V	12	301.6691	IV	0.5	258.6774	V	7	242.4323	V
18	375.0321	V	10	301.5910	IV	9	258.5813	IV	9	242.1939	V
20	374.8552	V	5	300.3830	IV	7	258.4167	V	10	242.1262	V
20	374.3670	V	5	300.3254	IV	7	258.4153	V	7	241.9258	V
20	374.2792	V	12	300.2727	IV	5	258.1836	IV	6	241.8694	V
50	374.0401	V	15	300.1237	IV	9	258.080	IV	8	241.7516	V
35	372.4206	V	9	299.2723	IV	9	258.0827	IV	7	241.3191	V
18	372.0153	V	10	298.9823	IV	1	258.007	IV	8	241.0945	V
9	371.2114	III	15	298.1187	IV	5	257.9519	V	7	241.0802	V
20	370.8995	V	8	297.3237	IV	8	257.575	IV	7	240.9593	V
18	369.4324	V	5	296.6941	IV	12	257.5490	V	8	239.4305	V
20	368.5296	V	9	296.6027	IV	9	257.5434	IV	1	239.0046	V
15	368.5034	V	10	295.8897	IV	8	257.3526	IV	9	238.7208	V
50	368.3239	V	8	295.3501	IV	7	256.5204	IV	8	238.2442	V
35	368.2901	V	8	293.3046	IV	3	256.2747	V	3	238.0113	V
25	367.9728	V	12	293.2161	IV	0.5	255.4346	V	6	237.363	V
25	364.2886	V	10	293.1653	IV	9	255.2500	V	6	237.139	V
20	363.7002	V	9	293.0687	IV	8	254.9877	V	8	236.5652	V
10	364.0494	IV	10	291.8004	IV	5	254.6422	V	9	236.2303	V
9	363.4916	III	12	291.1881	IV	15	254.5459	V	3	236.1874	V
25	361.2437	V	12	291.0897	IV	6	254.3651	V	8	234.9346	V
20	360.8256	V	10	290.5323	IV	8	253.5082	V	7	234.768	V
5	358.8008	III	10	289.6795	IV	9	253.3813	V	10	234.5671	V
9	357.0573	V	10	285.2983	IV	10	253.0161	V	8	234.339	V
12	356.9986	V	10	285.1680	IV	8	252.4234	V	2	234.0730	V
20	356.4761	V	10	285.0364	IV	10	252.1620	V	0.5	232.3395	V
20	356.1142	V	12	284.3115	IV	7	251.760	IV	2	231.6421	V
9	351.6203	III	7	283.1669	IV	8	251.690	IV	9	231.007	V
9	350.3240	V	9	283.0739	IV	12	251.6690	V	4	230.8388	V
7	349.9380	V	10	281.8157	IV	1	251.537	V	3	230.788	V
10	349.0276	V	10	274.7384	IV	5	251.4890	IV	5	230.5952	V
9	347.8310	V	2	274.3216	V	7	251.3692	V	0.5	230.4369	V
25	345.8811	V	6	271.3749	IV	6	251.2098	IV	8	228.334	V
18	343.1836	V	6	271.1892	IV	3	251.0671	IV	2	226.446	V
									6	224.083	V

Table VI. Comparison between observed and calculated energy-level values (in cm^{-1}) and calculated percentage compositions for the $4s4p^5 + 4s^24p^3(4d + 5d(+6d) + 5s + 6s(+7s))$ configurations of Sr V. Eigenvector components larger than 5% are given

<i>J</i>	<i>E</i> (obs.)	<i>E</i> (calc.)	Obs. – Calc.	Percentage composition
5	232 586	232 338	248	100(2D) $4d^3G$
	411 193	411 121	72	100(2D) $5d^3G$
4	202 913	202 511	402	96(4S) $4d^5D$
	224 844	224 435	409	72(3D) $4d^3F$ + 14(2P) $4d^3F$ + 10(2D) $4d^3G$
	230 974	230 773	201	76(3D) $4d^3G$ + 18(2D) $4d^3F$
	234 783	235 317	– 534	86(3D) $4d^1G$ + 6(2D) $4d^3G$
	251 234	251 053	181	74(2P) $4d^3F$ + 11(2D) $4d^1G$ + 7(3D) $4d^3G$
	386 847	386 950	– 103	95(4S) $5d^5D$
	408 238	408 037	200	54(3D) $5d^3G$ + 31(2D) $5d^1G$ + 13(2P) $5d^3F$
	410 365	410 650	– 285	66(3D) $5d^3F$ + 21(2D) $5d^1G$ + 12(3D) $5d^3G$
	411 153	410 973	180	40(2D) $5d^1G$ + 34(2D) $5d^3F$ + 26(2D) $5d^3G$
		430 505		82(2P) $5d^3F$ + 8(2D) $5d^3G$ + 7(2D) $5d^1G$
3	202 398	202 120	279	94(4S) $4d^5D$
	216 104	216 547	– 443	40(3D) $4d^3D$ + 38(4S) $4d^3D$ + 8(2D) $4d^3F$
	222 368	222 172	197	67(3D) $4d^3F$ + 13(2P) $4d^3F$ + 9(2D) $4d^3D$ + 6(4S) $4d^3D$
	229 950	229 788	161	86(3D) $4d^3G$ + 9(2D) $4d^3F$
	249 673	249 466	207	76(2P) $4d^3F$ + 12(2D) $4d^3F$ + 6(2D) $4d^3G$
	253 340	253 315	25	38(2P) $4d^3D$ + 33(2D) $4d^3D$ + 12(4S) $4d^3D$ + 8(2P) $4d^1F$
	266 239	266 897	– 658	54(2P) $4d^1F$ + 26(2D) $4d^1F$ + 14(2P) $4d^3D$
	271 500	271 530	– 30	38(4S) $4d^3D$ + 32(2P) $4d^3D$ + 14(3D) $4d^3D$ + 10(3D) $4d^1F$
	291 678	291 424	254	42(3D) $5s^3D$ + 32(2D) $4d^1F$ + 21(2P) $4d^1F$
	291 836	292 169	– 334	57(3D) $5s^3D$ + 23(2D) $4d^1F$ + 14(2P) $4d^1F$
	386 627	386 643	– 16	92(4S) $5d^3D$
	392 856	392 832	24	87(4S) $5d^3D$
	407 282	407 558	– 276	60(3D) $5d^3G$ + 22(2D) $5d^3F$ + 9(2P) $5d^3F$
	407 980	407 943	37	54(2D) $5d^3F$ + 24(2D) $5d^3G$ + 9(2D) $5d^3D$ + 6(2P) $5d^1F$ + 6(2P) $5d^3D$
	411 800	412 157	– 357	78(3D) $5d^3D$ + 13(2D) $5d^3F$
	417 658	417 936	– 278	80(3D) $5d^1F$
	426 317	426 425	– 107	95(2D) $6s^3D$
		427 108		63(2P) $5d^3F$ + 20(2P) $5d^3D$ + 8(2P) $5d^1F$
	433 203	433 214	– 11	41(2P) $5d^3D$ + 39(2P) $5d^1F$ + 7(2D) $5d^3F$
	433 660	433 409	252	39(2P) $5d^1F$ + 19(2P) $5d^3D$ + 18(2P) $5d^3F$ + 9(2D) $5d^1F$ + 7(2D) $5d^3G$
2	154 032	153 943	90	84(2S) p^5^3P + 11(2D) $4d^3P$
	202 321	202 124	198	96(4S) $4d^5D$
	213 784	213 918	– 134	31(4S) $4d^3D$ + 29(2D) $4d^3D$ + 18(3D) $4d^3F$ + 7(2P) $4d^1D$ + 7(2P) $4d^3F$
	220 550	220 507	43	57(3D) $4d^3F$ + 17(2D) $4d^3D$ + 13(2P) $4d^3F$ + 11(4S) $4d^3D$
	241 479	240 767	713	58(2P) $4d^1D$ + 22(2D) $4d^1D$ + 8(2P) $4d^3F$
	248 383	248 067	316	49(2P) $4d^3D$ + 24(2D) $4d^3D$ + 14(4S) $4d^3D$ + 6(2P) $4d^3F$
	250 657	250 630	27	63(2P) $4d^3F$ + 22(2D) $4d^3F$
	255 119	254 833	286	80(2P) $4d^3P$ + 7(2D) $4d^3P$
	266 325	265 936	389	70(4S) $5s^5S$ + 18(2D) $4d^3P$ + 5(2P) $5s^3P$
	267 351	267 962	– 611	56(3D) $4d^3P$ + 26(4S) $5s^5S$ + 9(2S) p^5^3P
	276 821	276 820	2	33(2P) $4d^3D$ + 30(4S) $4d^3D$ + 14(2D) $4d^3D$ + 10(2D) $4d^1D$
	285 450	285 895	– 445	59(2D) $4d^1D$ + 21(2P) $4d^1D$ + 7(2P) $4d^3D$ + 5(4S) $4d^3D$
	289 117	289 168	– 52	73(3D) $5s^3D$ + 13(2P) $5s^3P$ + 9(2D) $5s^1D$
	294 818	294 955	– 137	81(2D) $5s^1D$ + 14(2D) $5s^3D$
	311 700	311 802	– 102	78(2P) $5s^3P$ + 9(2D) $5s^1D$ + 9(2D) $5s^3D$
	386 582	386 556	25	93(4S) $5d^5D$
	391 773	391 734	38	81(4S) $5d^3D$ + 5(2D) $5d^3D$
	402 357	402 307	49	95(4S) $6s^5S$
	406 129	406 443	– 314	75(2D) $5d^3F$ + 7(2P) $5d^3F$
	410 517	410 580	– 63	42(2D) $5d^3D$ + 33(2D) $5d^3P$ + 10(2P) $5d^3P$
	413 008	413 039	– 31	44(3D) $5d^3D$ + 37(2D) $5d^3P$ + 9(2D) $5d^1D$
	415 542	415 425	117	66(2D) $5d^1D$ + 17(2D) $5d^3P$ + 6(2D) $5d^3F$
	423 316	423 347	– 32	63(3D) $6s^3D$ + 20(2D) $6s^1D$ + 14(2P) $6s^3P$
		426 071		73(2P) $5d^3F$ + 15(2P) $5d^1D$
	427 207	427 226	– 18	41(2P) $5d^3D$ + 32(2P) $5d^3P$ + 20(2P) $5d^1D$
	427 217	427 380	– 163	69(2D) $6s^1D$ + 24(2D) $6s^3D$
	431 700	431 804	– 104	50(2P) $5d^3P$ + 18(2P) $5d^1D$ + 10(2D) $5d^3P$ + 10(2P) $5d^3D$ + 6(2D) $5d^3D$
	433 958	433 910	48	30(2P) $5d^3D$ + 28(2P) $5d^1D$ + 13(2P) $5d^3F$ + 10(2D) $5d^1D$ + 10(2D) $5d^3F$
	446 263	446 236	27	81(2P) $6s^3P$ + 9(2D) $6s^3D$ + 7(2D) $6s^1D$
1	160 018	160 031	– 13	82(2S) p^5^3P + 11(2D) $4d^3P$
	193 319	193 228	91	58(2S) p^5^1P + 34(2D) $4d^1P$ + 5(2P) $4d^1P$
	202 265	202 112	153	97(4S) $4d^5D$
	216 969	217 765	– 796	47(3D) $4d^3D$ + 47(4S) $4d^3D$
	243 576	243 219	357	50(2P) $4d^3D$ + 35(2D) $4d^3D$ + 13(4S) $4d^3D$
	248 012	247 839	173	70(2P) $4d^3P$ + 20(2D) $4d^3P$

Table VI. Continued

<i>J</i>	<i>E</i> (obs.)	<i>E</i> (calc.)	Obs. – Calc.	Percentage composition
	265 179	264 255	924	88 (² <i>D</i>)4 <i>d</i> ³ <i>S</i> + 9 (² <i>D</i>)4 <i>d</i> ³ <i>P</i>
	269 615	269 899	– 285	33 (² <i>D</i>)4 <i>d</i> ³ <i>P</i> + 24 (² <i>D</i>)4 <i>d</i> ¹ <i>P</i> + 15 (² <i>S</i>) <i>p</i> ⁵ 1 <i>P</i> + 7 (² <i>P</i>)4 <i>d</i> ³ <i>P</i> + 6 (² <i>S</i>) <i>p</i> ⁵ 3 <i>P</i>
	274 952	274 888	64	84 (⁴ <i>S</i>)5 <i>s</i> ³ <i>S</i> + 5 (² <i>D</i>)4 <i>d</i> ³ <i>P</i>
	275 488	275 582	– 94	35 (² <i>D</i>)4 <i>d</i> ¹ <i>P</i> + 18 (² <i>D</i>)4 <i>d</i> ³ <i>P</i> + 16 (² <i>S</i>) <i>p</i> ⁵ 1 <i>P</i> + 13 (² <i>P</i>)4 <i>d</i> ³ <i>P</i> + 6 (² <i>S</i>) <i>p</i> ⁵ 3 <i>P</i>
	280 067	280 127	– 60	40 (² <i>P</i>)4 <i>d</i> ³ <i>D</i> + 31 (⁴ <i>S</i>)4 <i>d</i> ³ <i>D</i> + 14 (² <i>D</i>)4 <i>d</i> ³ <i>D</i>
	288 832	288 976	– 144	84 (² <i>D</i>)5 <i>s</i> ³ <i>D</i> + 6 (² <i>P</i>)5 <i>s</i> ¹ <i>P</i>
	306 075	305 926	150	66 (² <i>P</i>)4 <i>d</i> ¹ <i>P</i> + 18 (² <i>P</i>)5 <i>s</i> ³ <i>P</i>
	307 806	307 784	23	66 (² <i>P</i>)5 <i>s</i> ³ <i>P</i> + 18 (² <i>P</i>)4 <i>d</i> ¹ <i>P</i> + 9 (² <i>P</i>)5 <i>s</i> ¹ <i>P</i>
	314 736	314 578	157	76 (² <i>P</i>)5 <i>s</i> ¹ <i>P</i> + 11 (² <i>D</i>)5 <i>s</i> ³ <i>D</i> + 8 (² <i>P</i>)5 <i>s</i> ³ <i>P</i>
	386 568	386 530	38	95 (⁴ <i>S</i>)5 <i>d</i> ⁵ <i>D</i>
	392 708	392 638	70	89 (⁴ <i>S</i>)5 <i>d</i> ³ <i>D</i>
	404 878	404 804	74	93 (⁴ <i>S</i>)6 <i>s</i> ³ <i>S</i>
	408 586	408 422	164	49 (² <i>D</i>)5 <i>d</i> ³ <i>D</i> + 30 (² <i>D</i>)5 <i>d</i> ¹ <i>P</i> + 5 (² <i>P</i>)5 <i>d</i> ³ <i>D</i> + 5 (² <i>P</i>)5 <i>d</i> ³ <i>P</i>
	412 486	412 387	100	31 (² <i>D</i>)5 <i>d</i> ³ <i>S</i> + 29 (² <i>D</i>)5 <i>d</i> ¹ <i>P</i> + 17 (² <i>D</i>)5 <i>d</i> ³ <i>D</i> + 12 (² <i>D</i>)5 <i>d</i> ³ <i>P</i> + 7 (² <i>P</i>)5 <i>d</i> ³ <i>P</i>
	413 446	413 380	66	37 (² <i>D</i>)5 <i>d</i> ³ <i>P</i> + 24 (² <i>D</i>)5 <i>d</i> ³ <i>D</i> + 21 (² <i>D</i>)5 <i>d</i> ¹ <i>P</i> + 12 (² <i>D</i>)5 <i>d</i> ³ <i>S</i>
	414 775	414 558	217	46 (² <i>D</i>)5 <i>d</i> ³ <i>S</i> + 42 (² <i>D</i>)5 <i>d</i> ³ <i>P</i> + 10 (² <i>D</i>)5 <i>d</i> ¹ <i>P</i>
	423 108	423 128	– 21	84 (² <i>D</i>)6 <i>s</i> ³ <i>D</i> + 8 (² <i>P</i>)6 <i>s</i> ¹ <i>P</i>
	428 456	428 322	134	60 (² <i>P</i>)5 <i>d</i> ³ <i>D</i> + 25 (² <i>P</i>)5 <i>d</i> ³ <i>P</i> + 7 (² <i>P</i>)5 <i>d</i> ¹ <i>P</i>
	431 024	430 981	44	58 (² <i>P</i>)5 <i>d</i> ³ <i>P</i> + 21 (² <i>P</i>)5 <i>d</i> ³ <i>D</i> + 6 (² <i>D</i>)5 <i>d</i> ³ <i>S</i> + 5 (² <i>D</i>)5 <i>d</i> ¹ <i>P</i>
	438 713	438 887	– 175	74 (² <i>P</i>)5 <i>d</i> ¹ <i>P</i> + 5 (² <i>P</i>)5 <i>d</i> ³ <i>D</i>
	441 606	441 439	167	74 (² <i>P</i>)6 <i>s</i> ³ <i>P</i> + 24 (² <i>P</i>)6 <i>s</i> ¹ <i>P</i>
	447 043	447 052	9	63 (² <i>P</i>)6 <i>s</i> ¹ <i>P</i> + 19 (² <i>P</i>)6 <i>s</i> ³ <i>P</i> + 14 (² <i>D</i>)6 <i>s</i> ³ <i>D</i>
0	164 016	164 036	– 21	84 (² <i>S</i>) <i>p</i> ⁵ 3 <i>P</i> + 12 (² <i>D</i>)4 <i>d</i> ³ <i>P</i>
	202 129	201 988	140	97 (⁴ <i>S</i>)4 <i>d</i> ⁵ <i>D</i>
	221 778	223 791	– 2012	95 (² <i>D</i>)4 <i>d</i> ¹ <i>S</i>
	246 801	246 943	– 142	66 (² <i>P</i>)4 <i>d</i> ³ <i>P</i> + 27 (² <i>D</i>)4 <i>d</i> ³ <i>P</i>
	275 425	275 384	42	58 (² <i>D</i>)4 <i>d</i> ³ <i>P</i> + 24 (² <i>P</i>)4 <i>d</i> ³ <i>P</i> + 15 (² <i>S</i>) <i>p</i> ⁵ 3 <i>P</i>
	306 607	306 467	140	98 (² <i>P</i>)5 <i>s</i> ³ <i>P</i>
	386 525	386 504	21	95 (⁴ <i>S</i>)5 <i>d</i> ⁵ <i>D</i>
		408 560		82 (² <i>D</i>)5 <i>d</i> ¹ <i>S</i> + 9 (² <i>P</i>)5 <i>d</i> ³ <i>P</i> + 7 (² <i>D</i>)5 <i>d</i> ³ <i>P</i>
	413 822	413 822	1	85 (² <i>D</i>)5 <i>d</i> ³ <i>P</i> + 11 (² <i>D</i>)5 <i>d</i> ¹ <i>S</i>
	430 002	430 045	– 43	84 (² <i>P</i>)5 <i>d</i> ³ <i>P</i> + 6 (² <i>D</i>)5 <i>d</i> ³ <i>P</i> + 6 (² <i>D</i>)5 <i>d</i> ¹ <i>S</i>
		441 035		100 (² <i>P</i>)6 <i>s</i> ³ <i>P</i>

Mean error of the least-squares fit $\sigma = [\Sigma (E_{\text{obs}} - E_{\text{calc}})^2 / (N - P)]^{1/2} = 391 \text{ cm}^{-1}$ with $N = 95$ known levels and $P = 29$ adjustable parameters

Table VII. Energy parameters (in cm^{-1}) for $4s4p^5 + 4s^24p^3(4d + 5d + 6d + 5s + 6s + 7s)$ configurations of Sr V

Parameter	HF (E_{av})	Fitted	Fitted/HF
<i>p</i> ⁵			
E_{av}		188 856 ± 280	
$G^1(4s, 4p)$	97 058	76 817 ± 1030	0.791 ± 0.011
ζ_{4p}	6 347	6 983 ± 420	1.100 ± 0.066
<i>Ss</i>			
E_{av}		292 847 ± 140	
$F^2(4p, 4p)$	74 141	59 748 ± 970	0.806 ± 0.013
$G^1(4p, 5s)$	7 374	6 497 ± 420	0.881 ± 0.057
ζ_{4p}	6 751	7 713 ± 290	1.142 ± 0.043
<i>6s</i>			
E_{av}		426 790 ± 130	
$F^2(4p, 4p)$	74 596	60 685 ± 850	0.814 ± 0.011
$G^1(4p, 6s)$	2 349	2 004 ± 380	0.853 ± 0.160
ζ_{4p}	6 823	7 675 ± 260	1.125 ± 0.038
<i>7s</i>			
E_{av}		480 000 (fix)	
$F^2(4p, 4p)$	74 706	74 706 (fix)	1.0
$G^1(4p, 5s)$	1 099	1 099 (fix)	1.0
ζ_{4p}	6 843	6 843 (fix)	1.0
<i>4d</i>			
E_{av}		242 178 ± 70	
$F^2(4p, 4p)$	73 111	58 879 ± 560	0.805 ± 0.008
$F^2(4p, 4d)$	58 940	51 516 ± 560	0.874 ± 0.010
$G^1(4p, 4d)$	72 526	60 396 ± 220	0.833 ± 0.003
$G^3(4p, 4d)$	44 791	37 847 ± 740	0.845 ± 0.017

Table VII. Continued

Parameter	HF (E_{av})	Fitted	Fitted/HF
ζ_{4p}	6 523	7 470 $\pm$ 190	1.145 $\pm$ 0.029
ζ_{4d}	419	365 $\pm$ 110	0.871 $\pm$ 0.260
5d			
E_{av}		411 772 $\pm$ 80	
$F^2(4p, 4p)$	74 534	61 277 $\pm$ 540	0.822 $\pm$ 0.007
$F^2(4p, 5d)$	15 919	12 824 $\pm$ 1100	0.806 $\pm$ 0.069
$G^1(4p, 5d)$	9 903	5 905 $\pm$ 340	0.596 $\pm$ 0.034
$G^3(4p, 5d)$	7 075	3 274 $\pm$ 740	0.460 $\pm$ 0.100
ζ_{4p}	6 800	7 679 $\pm$ 180	1.129 $\pm$ 0.026
ζ_{5d}	124	206 $\pm$ 100	1.661 $\pm$ 0.810
6d			
E_{av}		478 000 (fix)	
$F^2(4p, 4p)$	74 681	74 681 (fix)	1.0
$F^2(4p, 6d)$	7 078	7 078 (fix)	1.0
$G^1(4p, 6d)$	3 863	3 863 (fix)	1.0
$G^3(4p, 6d)$	2 900	2 900 (fix)	1.0
ζ_{4p}	6 835	6 835 (fix)	1.0
ζ_{5d}	61	61 (fix)	1.0
Configuration interaction integrals			
p^5-5s			
$R^1(4p4p, 4s5s)$	3 749 (.093) ^a	3 749 (fix)	1.0
p^5-6s			
$R^1(4p4p, 4s6s)$	963 (.039)	963 (fix)	1.0
p^5-7s			
$R^1(4p4p, 4s7s)$	339 (.020)	339 (fix)	1.0
p^5-4d			
$R^1(4p4p, 4s4d)$	82 277 (.998)	62 482 (fix)	0.76
p^5-5d			
$R^1(4p4p, 4s5d)$	29 449 (.836)	22 234 (fix)	0.76
p^5-6d			
$R^1(4p4p, 4s6d)$	17 719 (.759)	13 478 (fix)	0.76
$5s-6s$			
$R^1(4p5s, 6s4p)$	4 025 (.366)	4 025 (fix)	1.0
$5s-7s$			
$R^1(4p5s, 7s4p)$	2 678 (.350)	2 678 (fix)	1.0
$5s-4d$			
$R^2(4p5s, 4p4d)$	-8 129 (-.269)	-8 129 (fix)	1.0
$R^1(4p5s, 4d4p)$	-712 (-.020)	-712 (fix)	1.0
$5s-5d$			
$R^2(4p5s, 4p5d)$	11 882 (.769)	11 882 (fix)	1.0
$R^1(4p5s, 5d4p)$	3 061 (.207)	3 061 (fix)	1.0
$5s-6d$			
$R^2(4p5s, 4p6d)$	8 807 (.836)	8 807 (fix)	1.0
$R^1(4p5s, 6d4p)$	2 521 (.256)	2 521 (fix)	1.0
$6s-7s$			
$R^1(4p6s, 7s4p)$	1 599 (.346)	1 599 (fix)	1.0
$6s-4d$			
$R^2(4p6s, 4p4d)$	-4 769 (-.267)	-4 769 (fix)	1.0
$R^1(4p6s, 4d4p)$	-1 422 (-.066)	-1 422 (fix)	1.0
$6s-5d$			
$R^2(4p6s, 4p5d)$	-99 (-.010)	-99 (fix)	1.0
$R^1(4p6s, 5d4p)$	1 153 (.129)	1 153 (fix)	1.0
$6s-6d$			
$R^2(4p6s, 4p6d)$	3 599 (.591)	3 599 (fix)	1.0
$R^1(4p6s, 6d4p)$	1 079 (.182)	1 079 (fix)	1.0
$7s-4d$			
$R^2(4p7s, 4p4d)$	-3 338 (-.268)	-3 338 (fix)	1.0
$R^1(4p7s, 4d4p)$	-1 233 (-.081)	-1 233 (fix)	1.0
$7s-5d$			
$R^2(4p7s, 4p5d)$	-339 (-.054)	-339 (fix)	1.0
$R^1(4p7s, 5d4p)$	626 (.100)	626 (fix)	1.0
$7s-6d$			
$R^2(4p7s, 4p6d)$	502 (.116)	502 (fix)	1.0
$R^1(4p7s, 6d4p)$	634 (.152)	634 (fix)	1.0
$4d-5d$			
$R^2(4p4d, 4p5d)$	16 517 (.682)	14 649 (fix)	0.89
$R^1(4p4d, 5d4p)$	24 431 (.805)	30 760 (fix)	1.26
$R^3(4p4d, 5d4p)$	15 931 (.873)	12 258 (fix)	0.77

Table VII. Continued

Parameter	HF (E_{av})	Fitted	Fitted/HF
4d-6d			
$R^2(4p4d, 4p6d)$	9 127 (.572)	8 093 (fix)	0.89
$R^1(4p4d, 6d4p)$	14 342 (.716)	18 050 (fix)	1.26
$R^3(4p4d, 6d4p)$	9 394 (.789)	7 229 (fix)	0.77
5d-6d			
$R^2(4p5d, 4p6d)$	8 385 (.866)	7 414 (fix)	0.89
$R^1(4p5d, 6d4p)$	6 134 (.717)	7 722 (fix)	1.26
$R^3(4p5d, 6d4p)$	4 479 (.870)	3 446 (fix)	0.77

^a The values in parentheses are a measure of the amount of cancellation which occurred in forming the integral. These numbers are the ratio of the true R^k value to an R^k value calculated using the absolute value of each wave-function.

Table VIII. Comparison between observed and calculated energy-level values (in cm^{-1}) and calculated percentage compositions for the $4s^24p^35p$ configuration of Sr V. Eigenvector components larger than 5% are given

J	$E(\text{obs.})$	$E(\text{calc.})$	Obs. - Calc.	Percentage composition
4	340 419	340 343	76	100 (2D) 3F
3	316 120	315 980	140	95 (4S) 5P
	336 623	336 518	105	67 (2D) 3F + 20 (2D) 3D + 10 (2P) 3D
	338 692	338 707	-15	60 (2D) 1F + 34 (2D) 3D
	339 930	339 962	-32	46 (2D) 3D + 30 (2D) 1F + 24 (2D) 3F
	359 647	359 619	28	81 (2P) 3D + 8 (2D) 3F + 8 (2D) 1F
2	314 143	314 011	132	84 (4S) 5P + 8 (4S) 3P
	321 239	321 367	-128	78 (4S) 3P + 12 (4S) 5P + 6 (2D) 3P
	334 365	334 280	84	48 (2D) 3F + 35 (2D) 3D + 10 (2P) 3D
	336 695	336 593	102	51 (2D) 3D + 37 (2D) 3F + 6 (2P) 1D
	343 583	343 816	-233	69 (2D) 3P + 12 (2P) 3P + 8 (4S) 3P + 6 (2D) 1D
	351 337	351 368	-31	73 (2D) 1D + 10 (2D) 3P + 5 (2P) 3D
	356 567	356 356	211	75 (2P) 3D + 10 (2P) 3P + 5 (2P) 1D
	362 487	362 536	-49	74 (2P) 1D + 8 (2D) 1D + 7 (2D) 3F
	364 887	364 958	-71	63 (2P) 3P + 9 (2D) 3P + 9 (2D) 1D + 8 (2P) 1D + 6 (2D) 3D
1	313 727	313 581	146	91 (4S) 5P
	319 835	319 825	10	73 (4S) 3P + 8 (2D) 3P + 6 (2P) 1P
	331 198	331 371	-173	40 (2D) 3D + 34 (2D) 1P + 9 (2P) 1P + 7 (4S) 3P
	337 454	337 657	-203	46 (2D) 1P + 41 (2D) 3D + 8 (2P) 3D
	345 344	345 468	-123	68 (2D) 3P + 14 (2P) 3S + 13 (4S) 3P
	353 845	353 763	82	73 (2P) 3D + 15 (2P) 1P + 6 (2D) 3D
	357 248	357 135	113	74 (2P) 3S + 18 (2D) 3P
	357 554	357 560	-5	65 (2P) 3P + 26 (2P) 1P + 5 (2P) 3D
	363 332	363 688	-356	40 (2P) 1P + 27 (2P) 3P + 10 (2D) 3D + 9 (2P) 3D + 8 (2D) 1P
0	321 641	321 713	-72	90 (4S) 3P
	345 057	345 172	-115	88 (2D) 3P + 8 (2P) 1S
	358 076	358 082	-6	91 (2P) 3P
	375 152	374 770	382	87 (2P) 1S + 7 (2D) 3P

Mean error of the least-squares fit $\sigma = [\Sigma(E_{\text{obs}} - E_{\text{calc}})^2/(N - P)]^{1/2} = 171 \text{ cm}^{-1}$ with $N = 28$ known levels and $P = 7$ adjustable parameters.

Table IX. Energy parameters (in cm^{-1}) for the $4s^24p^35p$ configuration of Sr V

Parameter	HF (E_{av})	Fitted	Fitted/HF
E_{av}		341 374 $\pm$ 33	
$F^2(4p, 4p)$	74 779	60 046 $\pm$ 241	0.803 $\pm$ 0.003
$F^2(4p, 5p)$	21 166	20 675 $\pm$ 315	0.977 $\pm$ 0.015
$G^0(4p, 5p)$	4 159	4 176 $\pm$ 33	1.004 $\pm$ 0.008
$G^2(4p, 5p)$	5 759	4 599 $\pm$ 257	0.799 $\pm$ 0.045
ζ_{4p}	6 848	7 649 $\pm$ 78	1.117 $\pm$ 0.011
ζ_{5p}	1 280	1 746 $\pm$ 74	1.364 $\pm$ 0.058

PAPER II

Spectrum of Rb IV

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Abstract

The Rb IV spectrum emitted from a sliding-spark discharge has been observed in the wavelength range 4500–290 Å. About 550 lines have been classified. From the observations 129 energy levels have been established in the $4s^2 4p^4$, $4s 4p^5$, $4s^2 4p^3 5s$, $6s$, $5p$, $4d$ and $5d$ configurations. The observed level structure has been interpreted by means of Hartree-Fock calculations and parametric fits including, in particular, Rydberg-series configuration interaction. The ionization energy of Rb^{3+} is estimated to be $421000 \pm 2000 \text{ cm}^{-1}$.

1. Introduction

Following a recent report on a study of the spectrum of the four-times ionized strontium atom [1] we are now reporting on an investigation of the preceding member of the Se I iso-electronic sequence, the three-times ionized rubidium atom. The first data on the Rb^{3+} ion were reported by Hansen and Persson [2] who studied the ground configuration, $4s^2 4p^4$, and the lowest excited configuration, $4s 4p^5$. In the present work the analysis has been extended to include the $4s^2 4p^3 5s$, $6s$, $5p$, $4d$ and $5d$ configurations. In all about 550 Rb IV lines have been classified.

The experimental observations have been interpreted by means of Hartree-Fock (HF) calculations and least-squares fits. Configuration-interaction (CI) effects, in particular Rydberg series CI, have been included in the calculations. As in Sr V the Rydberg series CI is found to have a substantial influence on the level distribution in the $4d$ configuration.

2. Experimental method

The rubidium spectrum was excited in a sliding spark between hollow beryllium electrodes carrying a rubidium salt. Three different compounds (RbCl , Rb_2SO_4 and Rb I) were used to facilitate a proper recognition of lines emanating from rubidium. Lines from different stages of ionization were recognized by studying the variation of line intensities as a function of the discharge current. In particular, a well developed Rb IV spectrum showed up at a peak current of around 300 A.

The observations cover the wavelength range 4500–290 Å. In the 4500–2000 Å range the spectrum was photographed on a 3.4 m Ebert-type plane-grating spectrograph while the region below 2500 Å was photographed on the 3 m normal-incidence [3] and 5 m grazing-incidence [4] spectrographs. The spectrograms were calibrated using internal standards, in particular Rb II [5], Rb III [6] and Cl II [7] lines and, in the region above 2000 Å, a superimposed spectrum from a Ne-Fe hollow-cathode discharge.

The classified Rb IV lines, in all about 550 lines, are given in Tables I–III. For unperturbed lines the uncertainty in the wavelength determination is $\pm 0.02 \text{ Å}$ above 2000 Å and $\pm 0.01 \text{ Å}$ below this limit. Below 500 Å the uncertainty is less than 0.005 Å.

3. Analysis

The Rb IV spectrum was analysed mainly in parallel with the Sr V spectrum [1]. The analysis comprises all levels of the $4s^2 4p^4$, $4s 4p^5$, $4s^2 4p^3 4d$ and $5s$ configurations, all but one of the levels of the $5p$ and $6s$ configurations and all but two of the $5d$ levels (Tables IV–V). The gross structure of the energy-level system is illustrated in Figure 1.

As in Sr V the electrostatic and magnetic interactions are of about the same magnitude and the coupling conditions in the excited configurations are intermediate. We have chosen to use *LS* designations for all levels.

3.1 Odd configurations

The level distributions in the $4s^2 4p^3 (4d + 5s)$ and $(5d + 6s)$ configurations are illustrated in Figures 2 and 3. The *nd* levels are marked by fully drawn lines, the *ns* levels by dashed lines. In the $5d + 6s$ group of levels the $(^2D)5d \ ^1S_0$, $(^2P)5d \ ^3F_4$ and $(^2P)6s \ ^3P_0$ levels have not been established experimentally.

To theoretically interpret the odd configurations we have used the approach described in detail in Ref. 1. The energy matrix used is the $4s 4p^5 + 4s^2 4p^3 (4d + 5d + 6d + 5s + 6s + 7s)$ matrix including CI, in particular Rydberg series CI [8], between all configurations involved. The experimentally unknown $6d$ and $7s$ levels were introduced in the calculation to account for, in an approximate way, the influence from higher-lying series members.

The Rydberg series CI was included in the calculation in an

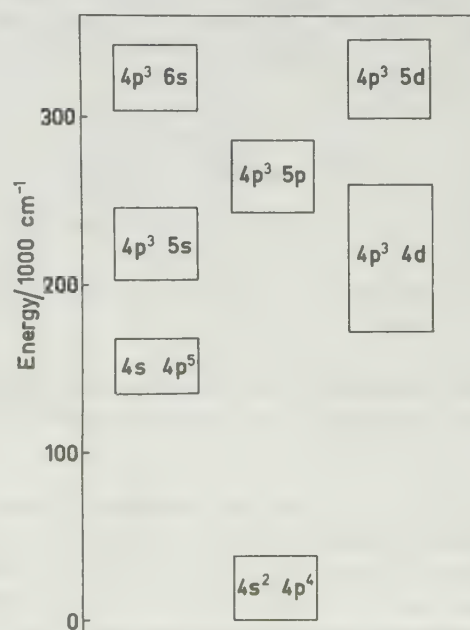


Fig. 1. Schematic diagram of the observed low configurations of Rb IV.

4. Ionization energy

The ionization energy of Rb IV has been estimated from an extrapolation to Rb IV of the variation of the quantum defects in the $ns(n = 5,6)$ and $nd(n = 4,5)$ series of Sr IV [11] and Zr IV [12, 13]. The value arrived at is $421000 \pm 2000 \text{ cm}^{-1}$.

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References

1. Persson, W. and Wahlström, C.-G., *Physica Scripta* **30**, 169 (1984).
2. Hansen, J. E. and Persson, W., *J. Opt. Soc. Am.* **64**, 696 (1974).
3. Minnhagen, L., *Physica Scripta* **11**, 38 (1975).
4. Lundström, T. and Minnhagen, L., *Physica Scripta* **5**, 243 (1972).
5. Reader, J. and Epstein, G. L., *J. Opt. Soc. Am.* **63**, 1153 (1973).
6. Hansen, J. E., Persson, W. and Valind, S., *Phys. Lett.* **42A**, 275 (1972).
7. Radziemski, L. J., Jr. and Kaufmann, V., *J. Opt. Soc. Am.* **64**, 366 (1974).
8. Cowan, R. D., *The Theory of Atomic Structure and Spectra*, Ch. 13. University of California Press (1981).
9. Moore, Ch. E., *Atomic Energy Levels*, Natl. Bur. Stand. Circ. 467, vol. II. Washington, 1952).
10. Persson, W. and Reader, J., Abstract to 16th EGAS, London (1984).
11. Persson, W., *Physica Scripta* **17**, 387 (1978).
12. Kiess, C. C., *J. Res. Natl. Bur. Stand.* **56**, 167 (1956).
13. Epstein, G. L. and Reader, J., *J. Opt. Soc. Am.* **65**, 310 (1975).

Table I. Observed combinations between excited states of Rb IV in the 4000–2500 Å range

Intensity and shape ^a	λ_{air} (Å)	σ (cm ⁻¹)		Classification ^b
		Obs.	Calc.	
5	3 943.369	25 351.85	2.57	(² P)4d ¹ P ₁ – (² P)5p ¹ D ₂
1	3 876.191	25 791.21	0.48	(² P)4d ¹ P ₁ – (² P)5p ¹ P ₁
3	3 599.042	27 777.24	.25	(² D)4d ³ P ₁ – (² D)5p ³ D ₁
5	3 556.512	28 109.40	.46	(² P)5s ¹ P ₁ – (² D)5p ¹ D ₂
9	3 441.555	29 048.31	.36	(² D)4d ¹ F ₃ – (² D)5p ¹ D ₂
5	3 349.201	29 849.29	.20	(² D)4d ³ P ₀ – (² D)5p ¹ P ₁
10	2 993.057	33 400.91	1.05	(² D)4d ³ D ₃ – (⁴ S)5p ³ P ₂
4	2 977.034	33 580.68	.70	(² D)4d ¹ D ₂ – (² D)5p ¹ D ₂
10	2 944.358	33 953.33	.35	(² D)5s ¹ D ₂ – (² D)5p ¹ P ₁
8	2 924.346	34 185.67	.67	(² D)5s ³ D ₂ – (² D)5p ³ D ₁
7	2 902.637	34 441.34	.34	(² D)5s ³ D ₁ – (² D)5p ³ D ₁
7	2 860.924	34 943.48	.57	(² P)4d ³ D ₃ – (² D)5p ¹ F ₃
15	2 851.594	35 057.80	.73	(² D)5s ¹ D ₂ – (² D)5p ¹ F ₃
6	2 839.583	35 206.09	.05	(² P)4d ³ P ₁ – (⁴ S)5p ³ P ₁
12	2 789.451	35 838.78	.86	(² D)5s ¹ D ₂ – (² D)5p ³ D ₃
10	2 777.512	35 992.83	.80	(² P)4d ¹ F ₃ – (² D)5p ³ F ₃
1	2 773.456	36 045.46	.37	(² P)5s ³ P ₂ – (² P)5p ³ D ₂
8	2 773.335	36 047.03	.18	(² P)4d ³ P ₁ – (⁴ S)5p ³ P ₂
6	2 771.045	36 076.81	.80	(² P)4d ³ D ₃ – (² D)5p ³ F ₄
10	2 752.336	36 322.04	1.92	(² P)5s ³ P ₂ – (² P)5p ³ S ₁
5	2 750.916	36 340.78	.81	(² P)4d ³ D ₂ – (⁴ S)5p ³ P ₁
8	2 737.537	36 518.39	.36	(² P)5s ³ P ₁ – (² P)5p ³ D ₁
12	2 716.825	36 796.76	.80	(² D)5s ³ D ₂ – (² D)5p ³ F ₂
7	2 701.378	37 007.16	.03	(² P)5s ³ P ₀ – (² P)5p ³ D ₁
8	2 698.079	37 052.42	.47	(² D)5s ³ D ₁ – (² D)5p ³ F ₂
12	2 693.224	37 119.21	.19	(⁴ S)5s ³ S ₁ – (⁴ S)5p ³ P ₁
10	2 679.341	37 311.52	.47	(² D)5s ³ D ₃ – (² D)5p ³ F ₃
8	2 654.601	37 659.23	.18	(² D)4d ³ P ₂ – (² D)5p ³ D ₃
2	2 638.954	37 882.51	1.45	(² D)5p ³ D ₂ – (⁴ S)5d ⁵ D ₂
10	2 633.546	37 960.31	.32	(⁴ S)5s ³ S ₁ – (⁴ S)5p ³ P ₂
12	2 621.461	38 135.28	.17	(² P)5s ³ P ₂ – (² P)5p ³ D ₃
10	2 620.121	38 154.80	5.02	(² P)5s ¹ P ₁ – (² P)5p ¹ D ₂
10	2 615.012	38 229.33	.32	(⁴ S)5s ³ S ₁ – (⁴ S)5p ³ P ₀
7	2 603.867	38 392.95	.90	(² P)4d ¹ F ₃ – (² D)5p ³ D ₃
15	2 600.750	38 438.97	.96	(² P)5s ³ P ₁ – (² P)5p ³ D ₂
15	2 600.625	38 440.81	.69	(² D)5s ³ D ₂ – (² D)5p ³ F ₃
6	2 595.931	38 510.31	.34	(² D)5s ³ D ₂ – (² D)5p ³ D ₂
8	2 590.374	38 592.92	.93	(² P)5s ¹ P ₁ – (² P)5p ¹ P ₁
20	2 587.039	38 642.66	.60	(⁴ S)5s ⁵ S ₂ – (⁴ S)5p ⁵ P ₁
3	2 582.166	38 715.59	.51	(² P)5s ³ P ₁ – (² P)5p ³ S ₁
15	2 580.206	38 745.00	.00	(² P)4d ¹ F ₃ – (² D)5p ³ F ₄
15	2 578.803	38 766.08	.01	(² D)5s ³ D ₁ – (² D)5p ³ D ₂
10	2 567.904	38 930.60	.44	(² D)5s ³ D ₃ – (² D)5p ¹ F ₃
25	2 565.098	38 973.19	.13	(⁴ S)5s ⁵ S ₂ – (⁴ S)5p ⁵ P ₂
10	2 557.171	39 094.00	3.92	(² D)4d ¹ F ₃ – (² P)5p ¹ D ₂
10	2 549.538	39 211.03	0.95	(² D)5s ³ D ₁ – (² D)5p ¹ P ₁
1	2 549.991	39 204.06	.18	(² P)5s ³ P ₀ – (² P)5p ³ S ₁
1	2 517.396	39 711.63	.57	(² D)5s ³ D ₃ – (² D)5p ³ D ₃
6	2 514.855	39 751.76	.75	(² P)5s ¹ P ₁ – (² P)5p ³ P ₂
8	2 508.154	39 857.96	8.09	(² P)5s ³ P ₀ – (² P)5p ³ P ₁
4	2 505.505	39 900.10	.20	(² P)5s ³ P ₁ – (² P)5p ³ P ₀
6	2 504.080	39 922.79	.84	(² P)4d ³ D ₁ – (⁴ S)5p ³ P ₁

^a Intensities are uncorrected visual estimates of the photographic densities of the lines.^b All levels are given in *LS* notation.

Table II. Observed combinations between excited states of Rb IV in the 2500–740 Å range

Intensity and shape ^a	$\lambda_{\text{vac.}}$ (Å)	$\sigma(\text{cm}^{-1})$		Classification ^b
		Obs.	Calc.	
18	2 496.270	40 059.8	.66	$(^2D)5s\ ^3D_2 - (^2D)5p\ ^1F_3$
25	2 496.022	40 063.7	.67	$(^2D)5s\ ^3D_3 - (^2D)5p\ ^3F_4$
25	2 484.696	40 246.4	.31	$(^4S)5s\ ^5S_2 - (^4S)5p\ ^5P_3$
8	2 448.538	40 840.7	.79	$(^2D)5s\ ^3D_2 - (^2D)5p\ ^3D_3$
7	2 441.362	40 960.8	.54	$(^2D)4d\ ^3P_2 - (^2D)5p\ ^3P_2$
2	2 437.067	41 032.9	.97	$(^2P)4d\ ^3D_1 - (^4S)5p\ ^3P_0$
2	2 425.767	41 224.1	.13	$(^2P)5s\ ^3P_2 - (^2P)5p\ ^1P_1$
5	2 420.516	41 313.5	.43	$(^2D)4d\ ^3D_2 - (^2D)5p\ ^1D_2$
10	2 398.412	41 694.3	.26	$(^2P)4d\ ^1F_3 - (^2D)5p\ ^3P_2$
9	2 372.606	42 147.8	.95	$(^2D)4d\ ^3P_2 - (^2D)5p\ ^3P_1$
10	2 359.450	42 382.8	.95	$(^2P)5s\ ^3P_2 - (^2P)5p\ ^3P_2$
9	2 324.889	43 012.8	.93	$(^2D)5s\ ^3D_3 - (^2D)5p\ ^3P_2$
0.5	2 315.899	43 179.8	.81	$(^2P)5s\ ^3P_1 - (^2P)5p\ ^1D_2$
m Rb III		43 231.	.17	$(^2D)4d\ ^3S_1 - (^2D)5p\ ^3P_2$
15	2 297.601	43 523.7	4.08	$(^2D)4d\ ^1P_1 - (^2P)5p\ ^3D_1$
2	2 292.647	43 617.7	.72	$(^2P)5s\ ^3P_1 - (^2P)5p\ ^1P_1$
0.5	2 292.201	43 626.2	.26	$(^2D)4d\ ^1D_2 - (^2P)5p\ ^1D_2$
0.5	2 284.163	43 779.7	.83	$(^4S)5s\ ^5S_2 - (^4S)5p\ ^3P_1$
4	2 269.413	44 064.3	.17	$(^2D)4d\ ^1D_2 - (^2P)5p\ ^1P_1$
9	2 265.410	44 142.1	.15	$(^2D)5s\ ^3D_2 - (^2D)5p\ ^3P_2$
0.5	2 241.103	44 620.9	.96	$(^4S)5s\ ^5S_2 - (^4S)5p\ ^3F_2$
0.5	2 206.070	45 329.5	.56	$(^2D)5s\ ^3D_2 - (^2D)5p\ ^3P_1$
1	2 204.068	45 370.6	.76	$(^2P)4d\ ^3P_2 - (^2D)5p\ ^3F_3$
7	2 202.887	45 395.0	4.97	$(^2D)5s\ ^1D_2 - (^2D)5p\ ^1D_2$
4 a Rb III	2 200.462	45 445.0	4.68	$(^2D)4d\ ^1P_1 - (^2P)5p\ ^3D_2$
8	2 199.612	45 462.6	.64	$(^2D)5s\ ^3D_1 - (^2D)5p\ ^3P_0$
8 b Rb III	2 193.712	45 584.8	5.23	$(^2D)5s\ ^3D_1 - (^2D)5p\ ^3P_1$
2	2 157.984	46 339.5	.58	$(^2D)5p\ ^1D_2 - (^2D)5d\ ^3D_2$
5	2 133.425	46 873.0	.65	$(^2D)4d\ ^3D_3 - (^2D)5p\ ^3F_2$
4	2 131.919	46 906.1	2.08	$(^2D)4d\ ^3P_0 - (^2P)5p\ ^3S_1$
5	2 117.962	47 215.2	5.92	$(^2D)4d\ ^1P_1 - (^2P)5p\ ^3P_0$
4	2 104.850	47 509.3	.29	$(^2D)4d\ ^3P_2 - (^2D)5p\ ^1D_2$
2	2 104.152	47 525.1	.41	$(^2P)4d\ ^3D_2 - (^2D)5p\ ^3D_1$
5	2 103.114	47 548.6	.99	$(^2D)4d\ ^3P_0 - (^2P)5p\ ^3P_1$
7	2 084.045	47 983.6	.60	$(^2D)4d\ ^3D_2 - (^2P)5p\ ^3P_1$
4	2 064.757	48 431.9	.54	$(^2D)4d\ ^3D_3 - (^2D)5p\ ^3F_3$
1	2 053.055	48 707.9	.85	$(^2D)4d\ ^3D_1 - (^2P)5p\ ^1D_2$
0.5	2 050.057	48 779.1	.94	$(^2D)4d\ ^3D_2 - (^2P)5p\ ^3D_3$
0.5	2 041.413	48 779.1	.08	$(^2D)5s\ ^1D_2 - (^2P)5p\ ^3D_1$
8	2 029.729	48 985.7	.78	$(^2P)4d\ ^3P_1 - (^2D)5p\ ^3F_2$
4	2 016.028	49 267.7	.68	$(^2D)5s\ ^3D_3 - (^2D)5p\ ^1D_2$
0.5	1 996.615	49 602.5	.51	$(^2D)4d\ ^3D_3 - (^2D)5p\ ^1F_3$
9	1 995.195	50 084.8	.81	$(^2D)5p\ ^3P_0 - (^2D)5d\ ^3D_1$
4	1 992.597	50 120.4	.54	$(^2P)4d\ ^3D_2 - (^2D)5p\ ^3F_2$
9	1 984.772	50 185.8	.53	$(^2D)4d\ ^1P_1 - (^2P)5p\ ^1D_2$
6	1 978.207	50 383.6	.64	$(^2D)4d\ ^3D_3 - (^2D)5p\ ^3D_3$
2	1 976.852	50 550.8	.79	$(^2D)5p\ ^1D_2 - (^2D)5d\ ^1D_2$
1	1 972.412	50 585.5	.52	$(^2P)4d\ ^3D_3 - (^2P)5p\ ^3D_2$
5	1 970.999	50 699.3	.32	$(^2P)4d\ ^3P_1 - (^2D)5p\ ^3D_2$
0.5	1 967.763	50 735.7	.68	$(^2D)5s\ ^1D_2 - (^2P)5p\ ^3D_2$
0.5	1 966.519	50 819.1	.74	$(^2D)4d\ ^3D_3 - (^2D)5p\ ^3F_4$
7	1 957.286	50 851.3	20.05	$(^4S)5p\ ^3P_2 - (^4S)5d\ ^5D_2$
2	1 955.248	50 851.3	.39	$(^4S)5p\ ^3P_2 - (^4S)5d\ ^5D_3$
6 b Rb II	1 945.273	51 091.2	.44	$(^2P)4d\ ^3D_1 - (^2D)5p\ ^3D_1$
1	1 945.273	51 144.4	.26	$(^2P)4d\ ^3P_1 - (^2D)5p\ ^1P_1$
4	1 936.858	51 406.7	.92	$(^2D)5p\ ^3P_1 - (^2D)5d\ ^3D_2$
4	1 935.677	51 630.0	.14	$(^2D)5s\ ^1D_2 - (^2P)5p\ ^3P_1$
6	1 929.236	51 661.5	.18	$(^4S)5p\ ^3P_1 - (^4S)5d\ ^5D_2$
4	1 918.214	51 834.0	.08	$(^2P)4d\ ^3D_2 - (^2D)5p\ ^3D_2$
4	1 911.759	52 131.8	.84	$(^2P)5p\ ^3P_2 - (^2P)5d\ ^3P_2$
8	1 907.858	52 307.9	.96	$(^2D)5p\ ^1D_2 - (^2D)6s\ ^1D_2$
7	1 898.424	52 414.8	.88	$(^2D)5p\ ^1D_2 - (^2D)5d\ ^1F_3$
0.5	1 883.834	52 675.3	.32	$(^2P)4d\ ^3D_3 - (^2P)5p\ ^3D_3$
6	1 876.581	53 083.2	.23	$(^2D)5p\ ^3P_0 - (^2D)5d\ ^1P_1$
		53 288.4	.56	$(^2D)5p\ ^3P_2 - (^2D)5d\ ^3D_3$

Table II (continued)

Intensity and shape ^a	$\lambda_{\text{vac.}}$ (Å)	$\sigma(\text{cm}^{-1})$		Classification ^b
		Obs.	Calc.	
1	1 874.665	53 342.9	.83	$(^2D)5p\ ^3F_4 - (^2D)5d\ ^3G_4$
4	1 873.238	53 383.5	.40	$(^2P)4d\ ^3D_2 - (^2D)5p\ ^1F_3$
7	1 867.379	53 551.0	0.92	$(^2P)5p\ ^3P_2 - (^2P)5d\ ^3D_3$
4	1 861.319	53 725.4	.15	$(^2D)5p\ ^3P_1 - (^2D)5d\ ^3F_1$
0.5	1 853.378	53 955.6	.62	$(^2D)5p\ ^3P_1 - (^2D)5d\ ^3P_0$
6	1 852.872	53 970.3	.64	$(^2D)5p\ ^1P_1 - (^2D)5d\ ^3F_2$
0.5	1 843.503	54 244.6	.66	$(^2P)5p\ ^3P_2 - (^2P)5d\ ^1F_3$
8	1 835.667	54 476.1	.06	$(^2D)5p\ ^1F_3 - (^2D)5d\ ^3G_4$
2	1 832.670	54 565.2	4.99	$(^2D)5p\ ^3P_1 - (^2D)6s\ ^3D_2$
6	1 832.430	54 572.4	.39	$(^2D)5s\ ^3D_3 - (^2P)5p\ ^3D_2$
2	1 831.172	54 609.8	.80	$(^2D)4d\ ^3P_2 - (^2P)5p\ ^3D_3$
7	1 830.285	54 636.3	.57	$(^2P)5p\ ^3P_1 - (^2P)5d\ ^3D_2$
7	1 829.223	54 668.0	7.66	$(^2D)5p\ ^3P_2 - (^2D)5d\ ^3P_2$
0.5	1 815.968	55 067.0	.18	$(^2D)4d\ ^3S_1 - (^2P)5p\ ^3S_1$
8	1 814.856	55 100.8	.86	$(^2D)5p\ ^3D_3 - (^2D)5d\ ^1G_4$
3	1 813.488	55 142.4	.24	$(^2P)5p\ ^3P_0 - (^2P)5d\ ^3D_1$
5	1 811.781	55 194.3	.70	$(^4S)5p\ ^5P_3 - (^4S)5d\ ^5D_2$
5	1 811.558	55 201.1	.09	$(^4P)5p\ ^1P_1 - (^2P)5d\ ^1D_2$
9	1 810.736	55 226.2	.04	$(^4S)5p\ ^5P_3 - (^4S)5d\ ^5D_3$
1	1 808.621	55 290.8	.48	$(^2P)5p\ ^3S_1 - (^2P)5d\ ^3D_2$
4	1 806.897	55 343.5	.52	$(^2P)4d\ ^1F_3 - (^2P)5p\ ^3D_3$
12	1 806.714	55 349.1	.09	$(^4S)5p\ ^5P_3 - (^4S)5d\ ^5D_4$
8	1 806.348	55 360.3	.33	$(^4P)5p\ ^3D_2 - (^2P)5d\ ^3F_3$
9	1 806.096	55 368.0	.14	$(^2D)5p\ ^3D_2 - (^2D)5d\ ^3G_3$
10	1 804.254	55 424.6	.57	$(^2D)5p\ ^3F_4 - (^2D)5d\ ^3G_5$
7	1 803.826	55 437.7	.79	$(^2D)5p\ ^3F_3 - (^2D)5d\ ^3G_3$
3	1 803.737	55 440.5	.53	$(^2D)5s\ ^1D_2 - (^2P)5p\ ^1D_2$
3	1 797.567	55 630.8	.77	$(^2D)4d\ ^3P_1 - (^2P)5p\ ^3P_2$
2	1 797.301	55 639.0	.00	$(^2P)5p\ ^1D_2 - (^2P)5d\ ^1D_2$
6	1 790.784	55 841.5	.39	$(^2P)5p\ ^1D_2 - (^2P)5d\ ^1F_3$
8	1 790.670	55 845.0	.01	$(^2D)5p\ ^3D_3 - (^2D)5d\ ^3F_4$
9	1 790.301	55 856.5	.56	$(^2D)5p\ ^3D_2 - (^2D)5d\ ^3F_3$
4	1 789.601	55 878.4	.44	$(^2D)5s\ ^1D_2 - (^2P)5p\ ^1P_1$
8	1 789.486	55 882.0	1.99	$(^2D)5p\ ^1F_3 - (^2D)5d\ ^1G_4$
6	1 788.887	55 900.7	.54	$(^4S)5p\ ^3P_2 - (^4S)5d\ ^3D_2$
9	1 782.692	56 094.9	5.03	$(^2D)5p\ ^3F_3 - (^2D)5d\ ^3G_4$
5	1 781.815	56 122.5	.54	$(^2D)5p\ ^3P_2 - (^2D)5d\ ^3S_1$
7	1 781.606	56 129.1	.12	$(^2D)5p\ ^3F_2 - (^2D)5d\ ^3F_2$
4	1 778.156	56 238.0	7.82	$(^2D)5p\ ^3F_4 - (^2D)5d\ ^3D_3$
7	1 778.008	56 242.7	.76	$(^4S)5p\ ^3P_0 - (^4S)5d\ ^3D_1$
0.5	1 775.215	56 331.2	.13	$(^2P)4d\ ^3P_1 - (^2D)5p\ ^3P_2$
8	1 771.531	56 448.4	.36	$(^4S)5p\ ^5P_2 - (^4S)5d\ ^5D_1$
9	1 770.943	56 467.1	.88	$(^4S)5p\ ^5P_2 - (^4S)5d\ ^5D_2$
10	1 769.936	56 499.2	.22	$(^4S)5p\ ^5P_2 - (^4S)5d\ ^5D_3$
8	1 767.956	56 562.5	.49	$(^2P)5p\ ^3D_1 - (^2P)5d\ ^3F_2$
4	1 767.104	56 589.8	.92	$(^2D)5p\ ^3D_3 - (^2D)5d\ ^3D_3$
1	1 766.581	56 606.5	.61	$(^4S)5p\ ^3P_2 - (^4S)6s\ ^5S_2$
10	1 766.038	56 623.9	.95	$(^4S)5p\ ^3P_2 - (^4S)5d\ ^3D_3$
6 a Rb IV	1 765.979	56 625.8	6.14	$(^2D)5p\ ^1F_3 - (^2D)5d\ ^3F_4$
6	1 765.786	56 632.0	.07	$(^2D)5s\ ^3D_2 - (^2P)5p\ ^3P_1$
9	1 762.378	56 741.5	.67	$(^4S)5p\ ^3P_1 - (^4S)5d\ ^3D_2$
8	1 761.806	56 759.9	.93	$(^4S)5p\ ^5P_1 - (^4S)5d\ ^5D_0$
8	1 761.218	56 778.9	.89	$(^4S)5p\ ^5P_1 - (^4S)5d\ ^5D_1$
8	1 760.607	56 798.6	.41	$(^4S)5p\ ^5P_1 - (^4S)5d\ ^5D_2$
8	1 756.751	56 923.3	.10	$(^2P)4d\ ^3D_3 - (^2P)5p\ ^3P_2$
9	1 751.871	57 081.8	.68	$(^2D)5p\ ^3F_2 - (^2D)5d\ ^3G_3$
2	1 751.334	57 099.3	.30	$(^2P)5p\ ^3P_2 - (^2P)6s\ ^3P_2$
1	1 747.874	57 212.4	.14	$(^2P)4d\ ^1D_2 - (^2D)5p\ ^3F_3$
7	1 743.590	57 352.9	.89	$(^4S)5p\ ^3P_1 - (^4S)5d\ ^3D_1$
7	1 743.035	57 371.2	.05	$(^2D)5p\ ^1F_3 - (^2D)5d\ ^3D_3$
7	1 742.282	57 396.0	5.95	$(^2P)4d\ ^3P_1 - (^2D)5p\ ^3P_0$
1	1 741.917	57 408.0	.03	$(^2P)5p\ ^3S_1 - (^2P)5d\ ^3P_0$
0.5	1 741.602	57 418.4	.52	$(^2D)5s\ ^3D_1 - (^2P)5p\ ^3P_0$
5	1 739.099	57 501.1	0.96	$(^2D)5p\ ^3F_3 - (^2D)5d\ ^1G_4$
8	1 738.568	57 518.6	.54	$(^2P)4d\ ^3P_1 - (^2D)5p\ ^3P_1$
7	1 737.012	57 570.1	.10	$(^2D)5p\ ^3F_2 - (^2D)5d\ ^3F_3$
9	1 732.300	57 726.7	.73	$(^2P)4d\ ^1D_2 - (^2D)5p\ ^1P_1$

Table II (continued)

Intensity and shape ^a	$\lambda_{\text{vac.}}$ (Å)	σ (cm ⁻¹)		Classification ^b
		Obs.	Calc.	
6	1 731.019	57 769.4	.35	(² D)5p ³ P ₂ — (² D)6s ³ D ₃
0.5	1 730.661	57 781.4	.53	(² P)5p ³ P ₂ — (² P)6s ¹ P ₁
7	1 730.145	57 798.6	.20	(² D)5p ¹ P ₁ — (² D)5d ³ D ₂
6	1 724.301	57 994.5	.70	(² P)5p ³ D ₃ — (² P)5d ³ D ₃
5	1 721.946	58 073.8	.57	(² P)4d ¹ F ₃ — (² P)5p ¹ D ₂
5	1 717.436	58 226.3	.82	(² P)5p ³ S ₁ — (² P)5d ³ P ₁
m Rb II		58 245.	.14	(² D)5p ³ D ₂ — (² D)5d ³ D ₂
1	1 709.545	58 495.1	.11	(² D)5p ³ F ₃ — (² D)5d ³ F ₄
0.5	1 708.702	58 524.0	4.98	(² D)5p ³ F ₂ — (² D)5d ³ D ₁
2	1 707.760	58 556.3	.08	(² P)5p ³ D ₁ — (² P)5d ³ D ₁
5	1 704.928	58 653.5	.31	(⁴ S)5p ³ P ₀ — (⁴ S)6s ³ S ₁
7	1 702.411	58 740.2	.30	(² P)4d ³ D ₂ — (² D)5p ³ P ₁
7	1 699.949	58 825.3	.25	(² D)5p ³ D ₁ — (² D)5d ³ F ₂
3	1 699.774	58 831.4	.31	(⁴ S)5p ³ P ₂ — (⁴ S)6s ³ S ₁
5 b Rb II	1 699.060	58 856.1	.11	(² P)4d ¹ D ₂ — (² D)5p ¹ F ₃
6	1 698.827	58 864.2	7.58	(² D)4d ³ P ₂ — (² P)5p ³ P ₂
6	1 697.208	58 920.3	.06	(² P)4d ³ P ₀ — (² D)5p ³ P ₁
6	1 695.204	58 990.0	.37	(² D)5p ³ D ₂ — (² D)5d ³ D ₃
8	1 686.936	59 279.1	.40	(² D)4d ³ F ₃ — (⁴ S)5p ³ P ₂
1	1 686.094	59 308.7	.02	(² D)5p ³ F ₃ — (² D)5d ³ D ₃
7	1 685.960	59 313.4	.18	(⁴ S)4d ³ D ₃ — (⁴ S)5p ³ P ₂
6	1 685.349	59 334.9	9.09	(⁴ S)5s ³ S ₁ — (² D)5p ³ P ₀
1	1 684.459	59 366.3	.24	(² D)5s ³ D ₃ — (² P)5p ¹ D ₂
0.5	1 682.610	59 431.5	.92	(² D)5p ¹ P ₁ — (² D)5d ¹ P ₁
5	1 679.076	59 556.6	.26	(² P)5p ¹ D ₂ — (² P)6s ¹ P ₁
1	1 677.507	59 612.3	.68	(⁴ S)5s ³ S ₁ — (² D)5p ³ P ₁
6	1 675.985	59 666.4	.66	(² D)4d ³ F ₂ — (⁴ S)5p ³ P ₁
6	1 671.268	59 834.8	.24	(² P)4d ¹ D ₂ — (² D)5p ³ D ₃
8	1 668.345	59 939.7	.44	(⁴ S)5p ³ P ₁ — (⁴ S)6s ³ S ₁
8 a	1 667.510	59 969.6	.89	(² D)5p ¹ F ₃ — (² D)6s ³ D ₂
0.5	1 663.708	60 106.7	.68	(² D)5p ³ F ₂ — (² D)5d ³ D ₂
3	1 660.602	60 219.1	.75	(² D)4d ³ D ₃ — (² D)5p ¹ D ₂
1	1 657.551	60 330.0	.39	(² D)4d ³ S ₁ — (² P)5p ¹ P ₁
4	1 656.486	60 368.8	.90	(² D)5p ³ D ₃ — (² D)5d ¹ D ₂
3	1 654.456	60 442.8	8.90	(² P)5p ³ D ₂ — (² P)6s ³ P ₁
1	1 651.466	60 552.3	29.90	(² D)5p ¹ P ₁ — (² D)5d ³ P ₀
2	1 647.198	60 709.2	9.12	(² D)5p ³ F ₃ — (² D)5d ³ P ₂
7	1 646.935	60 718.8	3.04	(⁴ S)4d ³ D ₂ — (⁴ S)5p ³ P ₁
5	1 641.770	60 909.9	.36	(⁴ S)4d ³ D ₃ — (⁴ S)5p ³ P ₃
9	1 639.847	60 981.3	.38	(² D)5p ¹ P ₁ — (² D)6s ³ D ₁
3	1 637.443	61 070.8	.61	(² D)5p ³ F ₄ — (² D)6s ³ D ₃
7	1 636.500	61 106.0	.97	(² D)5s ³ D ₃ — (² P)5p ³ P ₂
0.5	1 635.902	61 128.4	.26	(⁴ S)5p ⁵ P ₃ — (⁴ S)6s ⁵ S ₂
6	1 635.211	61 154.2	.71	(² D)5p ³ D ₃ — (² D)6s ³ D ₃
5	1 630.071	61 347.0	.11	(² D)5p ³ D ₁ — (² D)5d ³ D ₁
3	1 627.236	61 453.9	.21	(² D)4d ³ S ₁ — (² P)5p ³ P ₂
1	1 616.766	61 851.9	.32	(² D)5p ³ D ₂ — (² D)6s ³ D ₁
7	1 616.448	61 864.1	.08	(² P)5p ³ D ₃ — (² P)6s ³ P ₂
6	1 613.657	61 971.1	.86	(² D)5p ³ F ₃ — (² D)6s ³ D ₂
6	1 613.101	61 992.4	.84	(² D)5p ¹ F ₃ — (² D)6s ³ D ₃
4	1 609.975	62 112.8	.07	(² D)5p ³ D ₃ — (² D)6s ¹ D ₂
0.5	1 609.288	62 139.3	0.99	(² D)5p ³ D ₃ — (² D)5d ¹ F ₃
8	1 606.310	62 254.5	.41	(² D)5p ¹ P ₁ — (² D)5d ¹ D ₂
4	1 606.227	62 257.7	.74	(² P)4d ³ D ₁ — (² D)5p ³ P ₀
3	1 605.864	62 271.8	.50	(² P)5p ³ D ₁ — (² P)6s ³ P ₁
8	1 597.826	62 585.0	.44	(⁴ S)5p ⁵ P ₂ — (⁴ S)6s ⁵ S ₂
5	1 596.636	62 631.7	.91	(² D)5p ³ F ₂ — (² D)5d ³ P ₁
2	1 596.289	62 645.3	.78	(⁴ S)5p ⁵ P ₂ — (⁴ S)5d ³ D ₃
8 b	1 593.582	62 751.7	4.97	(⁴ S)5p ⁵ P ₁ — (⁴ S)6s ⁵ S ₂
			5.88	(² P)4d ³ P ₁ — (² D)5p ¹ D ₂
			.68	(² P)4d ³ P ₂ — (² P)5p ³ D ₂
			.20	(² D)5p ¹ F ₃ — (² D)6s ¹ D ₂
			2.12	(² D)5p ¹ F ₃ — (² D)5d ¹ F ₃

Table II (continued)

Intensity and shape ^a	$\lambda_{\text{vac.}}$ (Å)	$\sigma(\text{cm}^{-1})$		Classification ^b
		Obs.	Calc.	
9	1 589.617	62 908.2	.23	$(^2P)4d\ ^3P_2 - (^2P)5p\ ^3S_1$
0.5	1 586.327	63 038.7	9.09	$(^2D)4d\ ^1G_4 - (^2D)5p\ ^3F_3$
5	1 584.843	63 097.8	.75	$(^2D)5p\ ^3F_2 - (^2D)6s\ ^3D_2$
1	1 583.271	63 160.4	.33	$(^2P)5p\ ^3S_1 - (^2P)6s\ ^3P_2$
4	1 575.524	63 470.9	.81	$(^2D)5p\ ^3F_3 - (^2D)6s\ ^3D_3$
8	1 575.308	63 479.7	.58	$(^4S)4d\ ^3D_1 - (^4S)5p\ ^3P_1$
4 b	1 573.248	63 562.8	.14	$(^2P)4d\ ^3P_2 - (^2P)5p\ ^3P_1$
2	1 568.636	63 749.6	.58	$(^2D)5p\ ^1P_1 - (^2D)6s\ ^1D_2$
0.5	1 554.706	64 320.8	.71	$(^4S)4d\ ^3D_1 - (^4S)5p\ ^3P_2$
9	1 553.636	64 365.2	.15	$(^2P)4d\ ^3F_2 - (^2P)5p\ ^3D_1$
0.5	1 551.032	64 473.2	.14	$(^4S)5p\ ^3P_2 - (^4S)6s\ ^3S_1$
15 b C IV	1 548.207	64 590.9	89.71	$(^4S)4d\ ^3D_1 - (^4S)5p\ ^3P_0$
15	1 546.599	64 658.0	.06	$(^2D)4d\ ^1G_4 - (^2D)5p\ ^1F_3$
6	1 545.089	64 721.2	.48	$(^2P)4d\ ^3P_2 - (^2P)5p\ ^3D_3$
12	1 540.185	64 927.3	.01	$(^4S)4d\ ^3D_3 - (^4S)5p\ ^3P_2$
0.5	1 535.762	65 114.3	.70	$(^2D)5p\ ^3F_2 - (^2D)6s\ ^3D_3$
9	1 532.824	65 239.1	.09	$(^2D)4d\ ^3G_3 - (^2D)5p\ ^3F_2$
6	1 532.699	65 244.4	.46	$(^2D)4d\ ^3D_3 - (^2P)5p\ ^3D_2$
10	1 528.135	65 439.2	.19	$(^2D)4d\ ^1G_4 - (^2D)5p\ ^3D_3$
0.5	1 527.200	65 479.3	8.99	$(^2D)5p\ ^3D_1 - (^2D)6s\ ^3D_1$
10	1 524.842	65 580.6	.27	$(^4S)4d\ ^3D_2 - (^4S)5p\ ^3P_1$
4	1 521.868	65 708.7	.88	$(^2D)5p\ ^3D_1 - (^2D)6s\ ^3D_2$
5	1 519.949	65 791.7	.29	$(^2D)4d\ ^1G_4 - (^2D)5p\ ^3F_4$
10	1 510.483	66 204.0	3.92	$(^2D)4d\ ^3G_4 - (^2D)5p\ ^3F_3$
6	1 508.618	66 285.8	.75	$(^2P)4d\ ^3F_2 - (^2P)5p\ ^3D_2$
9	1 505.535	66 421.6	.40	$(^4S)4d\ ^3D_2 - (^4S)5p\ ^3P_2$
2	1 497.853	66 762.2	.02	$(^2D)5p\ ^3D_1 - (^2D)5d\ ^1D_2$
3	1 495.151	66 882.9	.98	$(^2D)4d\ ^3G_3 - (^2D)5p\ ^3F_3$
10	1 493.591	66 952.7	.63	$(^2D)4d\ ^3G_3 - (^2D)5p\ ^3D_2$
10	1 491.392	67 051.4	.34	$(^2P)4d\ ^3F_3 - (^2P)5p\ ^3D_2$
1	1 490.208	67 104.7	.75	$(^2P)4d\ ^3D_2 - (^2P)5p\ ^3D_1$
6	1 487.733	67 216.4	.21	$(^2P)4d\ ^3F_2 - (^2P)5p\ ^3P_1$
4	1 485.124	67 334.4	.26	$(^2D)4d\ ^3D_3 - (^2P)5p\ ^3D_3$
7	1 474.697	67 810.5	.44	$(^2P)4d\ ^3P_2 - (^2P)5p\ ^1P_1$
10	1 474.428	67 822.9	.89	$(^2D)4d\ ^3G_4 - (^2D)5p\ ^1F_3$
12	1 473.518	67 864.8	.78	$(^2P)4d\ ^3F_4 - (^2P)5p\ ^3D_3$
7	1 466.980	68 167.3	.14	$(^2P)4d\ ^3P_1 - (^2P)5p\ ^3S_1$
10	1 464.984	68 260.2	.15	$(^2D)4d\ ^3G_5 - (^2D)5p\ ^3F_4$
0.5	1 462.505	68 375.8	.55	$(^2P)4d\ ^3F_2 - (^2P)5p\ ^3D_3$
2	1 459.810	68 502.1	1.95	$(^2D)4d\ ^3G_3 - (^2D)5p\ ^1F_3$
10	1 457.642	68 604.0	.02	$(^2D)4d\ ^3G_4 - (^2D)5p\ ^3D_3$
7	1 449.917	68 969.5	.26	$(^2P)4d\ ^3P_2 - (^2P)5p\ ^3P_2$
7	1 446.318	69 141.1	.14	$(^2P)4d\ ^3F_3 - (^2P)5p\ ^3D_3$
7	1 445.747	69 168.4	.35	$(^2P)4d\ ^1D_2 - (^2D)5p\ ^1D_2$
1	1 443.353	69 283.1	.08	$(^2D)4d\ ^3G_3 - (^2D)5p\ ^3D_3$
2	1 441.923	69 351.8	.83	$(^2P)4d\ ^3P_1 - (^2P)5p\ ^3P_0$
5	1 438.590	69 512.5	.66	$(^2P)4d\ ^3P_0 - (^2P)5p\ ^3S_1$
7	1 435.120	69 680.6	.55	$(^2D)4d\ ^1S_0 - (^2D)5p\ ^3D_1$
8	1 429.474	69 955.8	.81	$(^2P)4d\ ^3D_2 - (^2P)5p\ ^3P_1$
6	1 428.871	69 985.3	.31	$(^2D)4d\ ^3D_3 - (^2P)5p\ ^1D_2$
0.5	1 427.968	70 029.6	8.98	$(^2D)5p\ ^3P_2 - (^2P)5d\ ^3P_2$
8	1 413.922	70 725.3	.26	$(^2D)4d\ ^3F_2 - (^2D)5p\ ^3D_1$
3	1 407.932	71 026.2	.60	$(^2P)4d\ ^3F_2 - (^2P)5p\ ^1D_2$
12	1 407.738	71 035.9	.55	$(^4S)4d\ ^5D_2 - (^4S)5p\ ^5P_1$
12	1 407.089	71 068.7	.60	$(^4S)4d\ ^5D_1 - (^4S)5p\ ^5P_1$
10	1 405.510	71 148.5	.41	$(^4S)4d\ ^5D_0 - (^4S)5p\ ^5P_1$
12	1 402.191	71 317.0	6.92	$(^4S)4d\ ^5D_3 - (^4S)5p\ ^5P_2$
12	1 401.221	71 366.3	.08	$(^4S)4d\ ^5D_2 - (^4S)5p\ ^5P_2$
10	1 400.578	71 399.1	.13	$(^4S)4d\ ^5D_1 - (^4S)5p\ ^5P_2$
6	1 399.295	71 464.6	.51	$(^2P)4d\ ^3F_2 - (^2P)5p\ ^1P_1$
8	1 396.999	71 582.0	.04	$(^2D)4d\ ^3D_3 - (^2P)5p\ ^3P_2$
10	1 396.592	71 602.9	.57	$(^2D)4d\ ^3F_4 - (^2D)5p\ ^3F_3$
3	1 392.912	71 792.1	.19	$(^2P)4d\ ^3F_3 - (^2P)5p\ ^1D_2$
10	1 391.615	71 859.0	.00	$(^2D)4d\ ^3F_3 - (^2D)5p\ ^3F_2$
15	1 383.468	72 282.1	.10	$(^4S)4d\ ^5D_4 - (^4S)5p\ ^5P_3$
12	1 377.596	72 590.2	.10	$(^4S)4d\ ^5D_3 - (^4S)5p\ ^5P_3$
8	1 376.671	72 639.0	.26	$(^4S)4d\ ^5D_2 - (^4S)5p\ ^5P_3$

Table II (continued)

Intensity and shape ^a	$\lambda_{\text{vac.}}$ (Å)	$\sigma(\text{cm}^{-1})$		Classification ^b
		Obs.	Calc.	
1	1 372.156	72 878.0	.28	$(^4S)5p\ ^3P_2 - (^2D)5d\ ^3D_2$
7	1 365.727	73 221.1	.54	$(^2D)4d\ ^3F_4 - (^2D)5p\ ^1F_3$
10	1 363.572	73 336.8	.39	$(^2D)4d\ ^3F_2 - (^2D)5p\ ^3F_2$
9	1 360.489	73 503.0	2.89	$(^2D)4d\ ^3F_3 - (^2D)5p\ ^3F_3$
4	1 359.836	73 538.3	7.84	$(^2P)4d\ ^3D_1 - (^2P)5p\ ^3P_1$
8	1 359.200	73 572.7	.51	$(^4S)5p\ ^3P_2 - (^2D)5d\ ^3D_3$
9	1 351.307	74 002.5	.54	$(^2D)4d\ ^3F_3 - (^2D)5p\ ^3D_2$
6	1 350.099	74 068.6	.67	$(^2D)4d\ ^3F_4 - (^2D)5p\ ^3D_3$
4	1 347.630	74 204.3	.62	$(^2P)4d\ ^3D_1 - (^2P)5p\ ^3P_0$
10	1 344.905	74 354.7	.11	$(^2P)4d\ ^3D_2 - (^2P)5p\ ^1P_1$
2	1 343.815	74 415.0	.77	$(^2D)4d\ ^3F_4 - (^2D)5p\ ^3F_4$
7	1 343.182	74 450.1	4.87	$(^2P)4d\ ^3P_0 - (^2P)5p\ ^1P_1$
6	1 342.768	74 473.0	.16	$(^2D)4d\ ^1S_0 - (^2D)5p\ ^1P_1$
8	1 339.613	74 648.4	.06	$(^2P)4d\ ^1D_2 - (^2P)5p\ ^3D_2$
2	1 334.195	74 951.6	.18	$(^4S)4d\ ^3D_1 - (^2D)5p\ ^3D_1$
8	1 333.682	74 980.4	.61	$(^4S)5p\ ^3P_2 - (^2D)5d\ ^3P_2$
0.5	1 331.171	75 121.8	.28	$(^2D)4d\ ^3F_2 - (^2D)5p\ ^3F_3$
12 b 3 × Rb IV	1 324.597	75 494.6	.86	$(^2D)4d\ ^3F_3 - (^2D)5p\ ^1F_3$
3	1 312.233	76 206.0	.87	$(^2D)4d\ ^3F_2 - (^2D)5p\ ^1P_1$
7 b C I	1 311.392	76 254.9	5.83	$(^4S)4d\ ^5D_1 - (^4S)5p\ ^3P_1$
1	1 310.865	76 285.5	5.09	$(^2D)4d\ ^3F_3 - (^2D)5p\ ^3F_4$
4	1 308.793	76 406.3	.64	$(^4S)4d\ ^5D_0 - (^4S)5p\ ^3P_1$
2 b 3 × Rb IV	1 305.500	76 599.0	.49	$(^4S)5p\ ^3P_2 - (^2D)5d\ ^3S_1$
7	1 302.948	76 749.0	.25	$(^2D)4d\ ^3F_2 - (^2D)5p\ ^1F_3$
6	1 299.299	76 964.6	8.87	$(^4S)4d\ ^3D_2 - (^2D)5p\ ^3D_1$
2	1 297.913	77 046.7	.75	$(^4S)4d\ ^5D_3 - (^4S)5p\ ^3P_2$
7	1 294.347	77 259.1	.96	$(^4S)4d\ ^5D_1 - (^4S)5p\ ^3P_2$
1	1 285.580	77 785.9	.31	$(^4S)4d\ ^3D_1 - (^2D)5p\ ^3F_2$
7	1 284.267	77 865.4	6.14	$(^2P)4d\ ^3D_1 - (^2P)5p\ ^1P_1$
1	1 265.085	79 046.1	.61	$(^4S)4d\ ^3D_3 - (^2D)5p\ ^3F_2$
7	1 262.409	79 213.7	.27	$4s4p\ ^5\ ^1P_1 - (^4S)5p\ ^3P_1$
5	1 259.169	79 417.5	.91	$(^2P)4d\ ^1D_2 - (^2P)5p\ ^1D_2$
6	1 256.610	79 579.2	.79	$(^4S)4d\ ^3D_1 - (^2D)5p\ ^1P_1$
5	1 255.469	79 651.5	.15	$(^4S)4d\ ^3D_3 - (^2D)5p\ ^3D_2$
1	1 239.443	80 681.4	.82	$(^2P)4d\ ^1D_2 - (^2P)5p\ ^1P_1$
6	1 234.509	81 003.9	.74	$(^2D)4d\ ^3F_2 - (^2D)5p\ ^3P_2$
6	1 233.446	81 073.7	.89	$(^4S)4d\ ^3D_2 - (^2D)5p\ ^3F_3$
6	1 226.719	81 518.3	.54	$(^4S)4d\ ^3D_2 - (^2D)5p\ ^3D_2$
8	1 220.860	81 909.5	.48	$(^4S)4d\ ^3D_2 - (^2D)5p\ ^1P_1$
5	1 210.327	82 622.3	.60	$(^4S)4d\ ^3D_3 - (^2D)5p\ ^3D_3$
2	1 108.464	90 214.9	.86	$(^4S)4d\ ^3D_2 - (^2D)5p\ ^1F_3$
5	1 052.802	94 984.7	.87	$4s4p\ ^5\ ^1P_1 - (^2D)5p\ ^3D_1$
0.5	1 038.514	96 291.5	.48	$4s4p\ ^5\ ^1P_1 - (^2D)5p\ ^1P_1$
2	939.619	106 426.1	.29	$(^4S)5p\ ^5P_1 - (^2P)5d\ ^3P_2$
0.5	788.863	126 764.7	.10	$4s4p\ ^5\ ^1P_1 - (^2D)5p\ ^1D_2$
7	783.858	127 574.2	.72	$4s4p\ ^5\ ^3P_0 - (^2D)5p\ ^3P_1$
2	777.797	128 568.3	5.89	$4s4p\ ^5\ ^3P_2 - (^2D)5p\ ^3D_2$
6	750.707	133 207.8	.28	$4s4p\ ^5\ ^3P_1 - (^2D)5p\ ^3P_2$
3	744.075	134 395.0	.70	$4s4p\ ^5\ ^3P_2 - (^2D)5p\ ^3P_2$
			.11	$4s4p\ ^5\ ^3P_2 - (^2D)5p\ ^3P_1$

^a Abbreviations for line characteristics: a = affected (by); b = blended (by); m = masked by. Intensities are uncorrected visual estimates of the photographic densities of the lines.

^b All levels are given in *LS* notation.

Table III. Observed resonance lines of Rb IV

Intensity and shape ^a	$\lambda_{\text{vac.}}$ (Å)	σ (cm ⁻¹)		Classification ^b
		Obs.	Calc.	
10	988.004	101 214.2	4.36	4s ² 4p ⁴ ¹ S ₀ — 4s5p ⁵ ³ P ₁
15	850.185	117 621.5	0.85	¹ D ₂ — 4s4p ⁵ ³ P ₂
9	817.924	122 260.8	0.27	¹ D ₂ — 4s4p ⁵ ³ P ₁
25	776.888	128 718.7	8.13	³ P ₁ — 4s4p ⁵ ³ P ₂
10	771.535	129 611.8	1.29	¹ S ₀ — 4s4p ⁵ ¹ P ₁
20	753.746	132 670.7	0.15	³ P ₀ — 4s4p ⁵ ³ P ₁
20	749.861	133 358.0	7.55	³ P ₁ — 4s4p ⁵ ³ P ₁
50	740.853	134 978.6	8.51	³ P ₂ — 4s4p ⁵ ³ P ₂
20	733.408	136 349.8	8.52	³ P ₁ — 4s4p ⁵ ³ P ₀
25	716.239	139 618.3	7.93	³ P ₂ — 4s4p ⁵ ³ P ₁
25	663.759	150 657.1	7.20	¹ D ₂ — 4s4p ⁵ ¹ P ₁
8	651.475	153 497.9	7.64	¹ D ₂ — (4S)4d ⁵ D ₁
3	651.331	153 531.7	0.69	¹ D ₂ — (4S)4d ⁵ D ₂
8	610.099	163 907.9	7.52	³ P ₀ — (4S)4d ⁵ D ₁
2	609.286	164 126.6	3.20	¹ D ₂ — (4S)4d ³ D ₂
9	607.841	164 516.8	5.11	³ P ₁ — (4S)4d ⁵ D ₀
8	607.546	164 596.6	4.92	³ P ₁ — (4S)4d ⁵ D ₁
0.5	603.793	165 619.8	7.59	¹ D ₂ — (4S)4d ³ D ₃
10	595.184	168 015.4	4.86	³ P ₂ — 4s4p ⁵ ¹ P ₁
9	585.289	170 855.8	5.30	³ P ₂ — (4S)4d ⁵ D ₁
10	585.176	170 888.7	8.35	³ P ₂ — (4S)4d ⁵ D ₂
10	585.006	170 938.4	7.51	³ P ₂ — (4S)4d ⁵ D ₃
9	582.669	171 624.1	4.20	¹ D ₂ — (2D)4d ³ F ₃
10	570.708	175 220.9	0.48	³ P ₁ — (4S)4d ³ D ₂
9	566.143	176 633.8	3.77	³ P ₀ — (4S)4d ³ D ₁
9	563.948	177 321.3	1.17	³ P ₁ — (4S)4d ³ D ₁
10	561.030	178 243.6	4.11	¹ D ₂ — (2D)4d ³ G ₃
10	551.741	181 244.6	4.09	³ P ₁ — (2D)4d ³ F ₂
10	551.022	181 481.0	0.86	³ P ₂ — (4S)4d ³ D ₂
3	548.575	182 290.5	88.80	³ P ₁ — (2D)4d ¹ S ₀
10	546.521	182 975.6	5.25	³ P ₂ — (4S)4d ³ D ₃
9	544.718	183 581.1	1.55	³ P ₂ — (4S)4d ³ D ₁
10	533.323	187 503.7	4.47	³ P ₂ — (2D)4d ³ F ₂
10	532.154	187 915.4	4.95	¹ D ₂ — (2P)4d ¹ D ₂
10	529.149	188 982.6	1.86	³ P ₂ — (2D)4d ³ F ₃
4	526.926	189 780.0	0.63	¹ D ₃ — (2P)4d ³ D ₁
0.5	517.164	193 362.1	2.66	¹ D ₂ — (2P)4d ³ D ₂
2	514.146	194 497.2	7.77	¹ D ₂ — (2P)4d ³ P ₁
9	511.936	195 337.0	6.67	¹ D ₂ — (2P)4d ³ F ₃
9	511.241	195 602.7	1.77	³ P ₂ — (2D)4d ³ G ₃
9	509.936	196 103.2	2.26	¹ D ₂ — (2P)4d ³ F ₂
2	507.553	197 023.6	0.92	³ P ₁ — (4S)5s ⁵ S ₂
8	507.244	197 143.9	3.55	¹ D ₂ — (2D)4d ³ D ₃
1	502.483	199 011.8	2.23	³ P ₁ — (2P)4d ¹ D ₂
15	499.523	200 191.0	0.56	³ P ₀ — (2P)4d ³ D ₁
15 b Rb III	497.821	200 875.3	7.91	³ P ₁ — (2P)4d ³ D ₁
12	492.623	202 995.0	4.16	³ P ₀ — (4S)5s ³ S ₁
15	491.929	203 281.3	1.30	³ P ₂ — (4S)5s ⁵ S ₂
12	490.961	203 682.2	1.56	³ P ₁ — (4S)5s ³ S ₁
10	489.596	204 250.0	49.18	³ P ₁ — (2P)4d ³ P ₀
18	489.092	204 460.4	59.94	³ P ₁ — (2P)4d ³ D ₂
10	488.024	204 908.0	7.30	³ P ₀ — (2P)4d ³ P ₁
6	487.155	205 273.4	2.61	³ P ₂ — (2P)4d ¹ D ₂
12	486.391	205 595.7	4.70	³ P ₁ — (2P)4d ³ P ₁
3	484.421	206 432.2	0.73	¹ D ₂ — (2D)5s ³ D ₁
1	483.822	206 687.4	6.40	¹ D ₂ — (2D)5s ³ D ₂
8	482.773	207 136.9	8.29	³ P ₂ — (2P)4d ³ D ₁
15	482.626	207 200.0	199.54	³ P ₁ — (2P)4d ³ F ₂
10	481.703	207 596.8	7.38	¹ D ₂ — (2D)4d ³ S ₁
12	481.195	207 816.0	5.62	¹ D ₂ — (2D)5s ³ D ₃
12	480.936	207 927.9	7.93	¹ S ₀ — (2P)5s ¹ P ₁
8	476.493	209 866.7	8.01	¹ D ₂ — (2D)4d ³ P ₂
20	476.321	209 942.3	1.94	³ P ₂ — (4S)5s ³ S ₁
12	474.262	210 853.7	3.61	³ P ₁ — (2P)4d ³ P ₂
18	472.393	211 688.3	8.33	¹ D ₂ — (2D)5s ¹ D ₂
7	472.138	211 802.5	2.49	¹ D ₂ — (2P)4d ³ D ₃
15	472.020	211 855.6	5.08	³ P ₂ — (2P)4d ³ P ₁

TABLE III (continued)

Intensity and shape ^a	$\lambda_{\text{vac.}}$ (Å)	$\sigma(\text{cm}^{-1})$		Classification ^b
		Obs.	Calc.	
15	470.158	212 694.3	4.33	$^3P_2 - (^2P)4d\ ^3F_3$
12	469.275	213 094.9	4.82	$^1D_2 - (^2D)4d\ ^3P_1$
20	466.197	214 501.5	1.24	$^3P_2 - (^2D)4d\ ^3D_3$
12	463.457	215 769.9	9.87	$^1D_2 - (^2D)4d\ ^3D_2$
12	461.170	216 839.6	40.61	$^3P_0 - (^2D)5s\ ^3D_1$
15	460.953	216 942.1	3.33	$^1D_2 - (^2D)4d\ ^1P_1$
12	460.587	217 114.2	3.99	$^3P_2 - (^2P)4d\ ^3P_2$
10	459.715	217 526.1	8.01	$^3P_1 - (^2D)5s\ ^3D_1$
10	459.172	217 783.4	3.68	$^3P_1 - (^2D)5s\ ^3D_2$
0.5	458.698	218 008.6	7.26	$^3P_0 - (^2D)4d\ ^3S_1$
18	457.254	218 696.6	4.66	$^3P_1 - (^2D)4d\ ^3S_1$
18	453.045	220 728.4	7.01	$^1D_2 - (^2D)4d\ ^3D_1$
18	452.562	220 964.1	30.38	$^1S_0 - (^2P)4d\ ^1P_1$
9	448.862	222 785.4	5.29	$^3P_1 - (^2D)4d\ ^3P_2$
			5.61	$^3P_1 - (^2D)5s\ ^1D_2$
20	447.420	223 503.7	2.60	$^1D_2 - (^2D)4d\ ^1D_2$
			4.70	$^3P_0 - (^2D)4d\ ^3P_1$
15	446.852	223 788.0	8.39	$^3P_2 - (^2D)5s\ ^3D_1$
10	446.529	223 949.6	9.05	$^1D_2 - (^2P)5s\ ^3P_1$
20 u	446.342	224 043.7	4.06	$^3P_2 - (^2D)5s\ ^3D_2$
15	446.048	224 191.2	2.10	$^3P_1 - (^2D)4d\ ^3P_1$
18	444.534	224 954.5	5.04	$^3P_2 - (^2D)4d\ ^3S_1$
20	444.100	225 174.4	3.28	$^3P_2 - (^2D)5s\ ^3D_3$
12	441.809	226 342.2	2.64	$^1D_2 - (^2P)5s\ ^3P_2$
20	441.519	226 491.0	1.95	$^3P_2 - (^2P)4d\ ^1F_3$
18	440.788	226 866.4	7.15	$^3P_1 - (^2D)4d\ ^3D_2$
15	440.744	226 889.0	9.76	$^3P_1 - (^2D)4d\ ^3P_0$
25	440.093	227 225.0	5.67	$^3P_2 - (^2D)4d\ ^3P_2$
15	439.847	227 351.8	3.21	$^3P_0 - (^2D)4d\ ^1P_1$
25	438.531	228 033.8	34.94	$^1D_2 - (^2D)4d\ ^1F_3$
			40.61	$^3P_1 - (^2D)4d\ ^1P_1$
15	436.595	229 045.2	5.99	$^3P_2 - (^2D)5s\ ^1D_2$
12	436.478	229 106.6	6.89	$^3P_0 - (^2D)4d\ ^3D_1$
30	436.377	229 159.5	60.15	$^3P_2 - (^2P)4d\ ^3D_3$
15	435.170	229 795.3	4.29	$^3P_1 - (^2D)4d\ ^3D_1$
18	433.929	230 452.6	2.48	$^3P_2 - (^2D)4d\ ^3P_1$
12	428.952	233 126.6	7.53	$^3P_2 - (^2D)4d\ ^3D_2$
10	426.333	234 558.2	7.66	$^3P_1 - (^2P)5s\ ^3P_0$
12	426.258	234 599.6	9.88	$^3P_1 - (^2D)4d\ ^1D_2$
9	425.445	235 048.2	6.33	$^3P_1 - (^2P)5s\ ^3P_1$
4	423.629	236 055.7	4.67	$^3P_2 - (^2D)4d\ ^3D_1$
4	421.156	237 441.5	39.92	$^3P_1 - (^2P)5s\ ^3P_3$
7	416.542	240 071.9	1.12	$^3P_1 - (^2P)5s\ ^1P_1$
1	415.177	240 861.0	0.26	$^3P_2 - (^2D)4d\ ^1D_2$
8	414.410	241 307.2	6.71	$^3P_2 - (^2P)5s\ ^3P_1$
12	410.348	243 695.9	700.30	$^3P_2 - (^2P)5s\ ^3P_2$
0.5	351.254	284 694.6	5.20	$^1S_0 - (^2D)5d\ ^3P_1$
2	350.500	285 306.4	5.15	$^1S_0 - (^2D)6s\ ^3D_1$
3	349.107	286 445.0	5.14	$^1D_2 - (^4S)5d\ ^3D_2$
9	348.227	287 168.7	8.55	$^1D_2 - (^4S)5d\ ^3D_3$
1	345.535	289 370.0	69.91	$^1D_2 - (^4S)6s\ ^3S_1$
2	341.925	292 462.0	1.93	$^3P_1 - (^4S)5d\ ^5D_2$
18	336.174	297 465.3	6.24	$^3P_0 - (^4S)5d\ ^3D_1$
20	336.087	297 541.9	2.42	$^3P_1 - (^4S)5d\ ^3D_2$
0.5	335.634	297 944.0	5.58	$^1S_0 - (^2P)5d\ ^3D_1$
15	335.397	298 153.9	3.64	$^3P_1 - (^4S)5d\ ^3D_1$
0.5	335.293	298 247.1	8.49	$^3P_1 - (^4S)6s\ ^5S_2$
1	334.781	298 703.0	2.79	$^3P_2 - (^4S)5d\ ^5D_1$
2	334.759	298 722.3	2.31	$^3P_2 - (^4S)5d\ ^5D_2$
0.5	333.764	299 612.9	2.32	$^1D_2 - (^2D)5d\ ^3F_2$
0.5	333.675	299 692.5	2.47	$^1S_0 - (^2P)5d\ ^3P_1$
10	333.578	299 779.9	9.79	$^3P_0 - (^4S)6s\ ^3S_1$
12	332.815	300 467.1	7.19	$^3P_1 - (^4S)6s\ ^3S_1$
7	332.707	300 564.7	4.88	$^1D_2 - (^2D)5d\ ^3G_3$

Table III (continued)

Intensity and shape ^a	$\lambda_{\text{vac.}}$ (Å)	σ (cm ⁻¹)		Classification ^b
		Obs.	Calc.	
6	332.167	301 053.7	3.30	$^1D_2 - (^2D)5d\ ^3F_3$
3	331.609	301 560.4	1.00	$^1S_0 - (^2P)6s\ ^3P_1$
10	331.150	301 978.2	8.18	$^1D_2 - (^2D)5d\ ^3D_1$
5	329.574	303 422.3	2.88	$^1D_2 - (^2D)5d\ ^3D_2$
18	329.161	303 802.6	2.80	$^3P_2 - (^4S)5d\ ^3D_2$
0.5	328.821	304 117.3	7.11	$^1D_2 - (^2D)5d\ ^3D_3$
6	328.499	304 415.1	4.02	$^3P_2 - (^4S)5d\ ^3D_1$
30	328.380	304 525.3	6.21	$^3P_2 - (^4S)5d\ ^3D_3$
12	327.894	304 976.8	6.60	$^1D_2 - (^2D)5d\ ^1P_1$
10	327.387	305 449.3	9.21	$^1S_0 - (^2P)6s\ ^1P_1$
5	327.336	305 496.3	6.21	$^1D_2 - (^2D)5d\ ^3P_2$
9	327.074	305 741.3	1.11	$^1D_2 - (^2D)5d\ ^3P_1$
10	326.178	306 581.4	0.95	$^1D_2 - (^2D)6s\ ^3D_2$
15 a Rb IV	326.052	306 700.0	0.0	$^1S_0 - (^2P)5d\ ^1P_1$
15 a Rb IV	326.023	306 727.0	7.57	$^3P_2 - (^4S)6s\ ^3S_1$
10	325.785	306 950.5	1.09	$^1D_2 - (^2D)5d\ ^3S_1$
18	325.062	307 634.1	4.09	$^1D_2 - (^2D)5d\ ^1D_2$
18	323.215	309 391.3	1.26	$^1D_2 - (^2D)6s\ ^1D_2$
20	323.104	309 498.0	8.18	$^1D_2 - (^2D)5d\ ^1F_3$
10	321.844	310 709.7	9.60	$^3P_1 - (^2D)5d\ ^3F_2$
12	320.115	312 387.8	8.06	$^3P_0 - (^2D)5d\ ^3D_1$
2	319.411	313 076.0	5.46	$^3P_1 - (^2D)5d\ ^3D_1$
18	317.945	314 520.2	0.16	$^3P_1 - (^2D)5d\ ^3D_2$
12	317.071	315 387.0	6.48	$^3P_0 - (^2D)5d\ ^1P_1$
5	316.381	316 074.3	3.88	$^3P_1 - (^2D)5d\ ^1P_1$
6	316.305	316 151.0	0.99	$^3P_0 - (^2D)5d\ ^3P_1$
12	315.695	316 761.4	0.94	$^3P_0 - (^2D)6s\ ^3D_1$
15	315.618	316 838.9	8.39	$^3P_1 - (^2D)5d\ ^3P_1$
10	315.488	316 969.3	9.98	$^3P_2 - (^2D)5d\ ^3F_2$
9	315.428	317 029.7	9.90	$^1D_2 - (^2P)5d\ ^3F_2$
12	315.390	317 068.3	8.86	$^3P_1 - (^2D)5d\ ^3P_0$
4	315.098	317 361.8	0.97	$^3P_0 - (^2D)5d\ ^3S_1$
10	315.012	317 448.3	8.34	$^3P_1 - (^2D)6s\ ^3D_1$
12	314.784	317 678.2	8.23	$^3P_1 - (^2D)6s\ ^3D_2$
9	314.717	317 746.1	8.34	$^1D_2 - (^2P)5d\ ^3F_3$
15	314.543	317 921.6	2.54	$^3P_2 - (^2D)5d\ ^3G_3$
9	314.513	317 952.0	5.04	$^1D_2 - (^2P)5d\ ^3D_2$
0.5	314.419	318 046.6	8.37	$^3P_1 - (^2D)5d\ ^3S_1$
8	314.061	318 410.0	0.96	$^3P_2 - (^2D)5d\ ^3F_3$
9	313.744	318 731.2	1.37	$^3P_1 - (^2D)5d\ ^1D_2$
8	313.150	319 336.0	5.84	$^3P_2 - (^2D)5d\ ^3D_1$
9	312.024	320 488.1	8.54	$^3P_1 - (^2D)6s\ ^1D_2$
7	311.781	320 738.5	8.38	$^1D_2 - (^2P)5d\ ^3P_1$
8	311.738	320 781.7	0.54	$^3P_2 - (^2D)5d\ ^3D_2$
0.5	311.664	320 858.7	7.53	$^1D_2 - (^2P)5d\ ^3P_2$
20	311.067	321 474.7	4.77	$^3P_2 - (^2D)5d\ ^3D_3$
12	310.293	322 276.6	6.51	$^1D_2 - (^2P)5d\ ^3D_3$
10	310.236	322 334.9	4.26	$^3P_2 - (^2D)5d\ ^1P_1$
8	309.975	322 607.2	6.91	$^1D_2 - (^2P)6s\ ^3P_1$
12	309.820	322 768.0	7.86	$^1D_2 - (^2P)5d\ ^1D_2$
20	309.738	322 853.4	3.87	$^3P_2 - (^2D)5d\ ^3P_2$
18	309.626	322 969.9	70.25	$^1D_2 - (^2P)5d\ ^1F_3$
9	309.503	323 098.8	8.77	$^3P_2 - (^2D)5d\ ^3P_1$
0.5	308.919	323 709.5	8.72	$^3P_2 - (^2D)6s\ ^3D_1$
8	308.700	323 939.0	8.61	$^3P_2 - (^2D)6s\ ^3D_2$
15	308.348	324 308.9	8.75	$^3P_2 - (^2D)5d\ ^3S_1$
9	306.914	325 824.7	4.89	$^1D_2 - (^2P)6s\ ^3P_2$
15	306.790	325 955.7	5.68	$^3P_2 - (^2D)6s\ ^3D_3$
9	306.283	326 495.0	5.12	$^1D_2 - (^2P)6s\ ^1P_1$
9	305.945	326 856.3	5.84	$^3P_2 - (^2D)5d\ ^1F_3$
0.5	304.761	328 126.3	7.18	$^3P_1 - (^2P)5d\ ^3F_2$
12	303.903	329 052.0	2.32	$^3P_1 - (^2P)5d\ ^3D_2$
12	303.581	329 400.9	1.37	$^3P_0 - (^2P)5d\ ^3D_1$
1	302.949	330 088.9	8.77	$^3P_1 - (^2P)5d\ ^3D_1$
10	301.960	331 169.3	9.87	$^3P_1 - (^2P)5d\ ^3P_0$
12	301.354	331 835.6	5.66	$^3P_1 - (^2P)5d\ ^3P_1$
6	301.246	331 955.2	4.81	$^3P_1 - (^2P)5d\ ^3P_2$

Table III (continued)

Intensity and shape ^a	$\lambda_{\text{vac.}}$ (Å)	σ (cm ⁻¹)		Classification ^b
		Obs.	Calc.	
8	300.285	333 016.9	6.79	³ P ₀ — (² P)6s ³ P ₁
5	299.935	333 406.0	6.0	³ P ₁ — (² P)6s ³ P ₀
2	299.666	333 704.5	4.19	³ P ₁ — (² P)6s ³ P ₁
12	299.522	333 865.6	5.14	³ P ₁ — (² P)5d ¹ D ₂
8	298.413	335 106.0	6.00	³ P ₂ — (² P)5d ³ F ₃
10 u	296.805	336 922.0	2.17	³ P ₁ — (² P)6s ³ P ₂
3	295.776	338 093.8	6.04	³ P ₂ — (² P)5d ³ P ₁
9	295.668	338 217.4	5.19	³ P ₂ — (² P)5d ³ P ₂
12	294.435	339 633.7	4.17	³ P ₂ — (² P)5d ³ D ₃
2	294.150	339 963.2	4.57	³ P ₂ — (² P)6s ³ P ₁
1	294.009	340 125.8	5.52	³ P ₂ — (² P)5d ¹ D ₂
0.5	293.834	340 328.0	7.91	³ P ₂ — (² P)5d ¹ F ₃
9	291.390	343 182.6	2.55	³ P ₂ — (² P)6s ³ P ₂

^a Abbreviations for line characteristics: a = affected by; b = blended by; u = unsymmetrical. Intensities are uncorrected visual estimates of the photographic densities of the lines.
^b All levels are given in *LS* notation.

Table IV. Even energy levels of Rb IV

Designation	E (cm ⁻¹)	Purity (%)
4s ² 4p ⁴	³ P ₂ 0.00	(95)
	³ P ₁ 6 260.38	(100)
	³ P ₀ 6 947.78	(94)
	¹ D ₂ 17 357.66	(95)
	¹ S ₀ 38 403.57	(94)
4s ² 4p ³ (⁴ S)5p	⁵ P ₃ 243 527.61	(96)
	⁵ P ₂ 242 254.43	(89)
	⁵ P ₁ 241 923.90	(94)
	³ P ₂ 247 902.26	(83)
	³ P ₁ 247 061.13	(80)
	³ P ₀ 248 171.26	(91)
	(² D)5p ³ F ₄ 265 236.95	(100)
	³ F ₃ 262 484.75	(66)
	³ F ₂ 260 840.86	(45)
	³ D ₃ 264 884.85	(36)
	³ D ₂ 262 554.40	(47)
	³ D ₁ 258 229.73	(42)
	³ P ₂ 268 186.21	(74)
	³ P ₁ 269 373.62	(75)
	³ P ₀ 269 251.03	(89)
	¹ F ₃ 264 103.72	(52)
	¹ D ₂ 274 440.96	(79)
	¹ P ₁ 262 999.34	(47)
	(² P)5p ³ D ₃ 281 835.47	(84)
(2P)5p	³ D ₂ 279 745.67	(79)
	³ D ₁ 277 825.07	(76)
	³ P ₂ 286 083.25	(67)
	³ P ₁ 280 676.13	(62)
	³ P ₀ 281 206.91	(94)
	³ S ₁ 280 022.22	(77)
	¹ D ₂ 284 486.52	(78)
	¹ P ₁ 284 924.43	(40)
	¹ S ₀	

Table V. Odd energy levels of Rb IV

Designation	$E(\text{cm}^{-1})$	Purity (%)		
$4s4p^5$	3P_2	134 978.51 (82)		
	3P_1	139 617.93 (81)		
	3P_0	142 608.90 (82)		
	1P_1	168 014.86 (52)		
	$n = 5$		$n = 6$	
$4s^24p^3(^4S)ns$	5S_2	203 281.30 (96)	304 508.87 (96)	
	3S_1	209 941.94 (78)	306 727.57 (96)	
	$(^2D)ns$ 3D_3	225 173.28 (64)	325 955.56 (98)	
	3D_2	224 044.06 (64)	323 938.61 (60)	
	3D_1	223 788.39 (54)	323 708.72 (70)	
	1D_2	229 045.99 (76)	326 748.92 (74)	
	$(^2P)ns$ 3P_2	243 700.30 (78)	343 182.55 (83)	
	3P_1	241 306.71 (72)	339 964.57 (74)	
	3P_0	240 818.04 (72)		
	1P_1	246 331.50 (72)	343 852.78 (64)	
	$n = 4$		$n = 5$	
$4s^24p^3(^4S)nd$	5D_4	171 245.51 (96)	298 876.70 (96)	
	5D_3	170 937.51 (95)	298 753.65 (94)	
	5D_2	170 888.35 (97)	298 722.31 (95)	
	5D_1	170 855.30 (97)	298 702.79 (96)	
	5D_0	170 775.49 (97)	298 683.83 (96)	
	3D_3	182 975.25 (41)	304 526.21 (85)	
	3D_2	181 480.86 (36)	303 802.80 (81)	
	3D_1	183 581.55 (50)	304 414.02 (87)	
	$(^2D)nd$ 3G_5	196 976.80 (100)	320 661.52 (100)	
	3G_4	196 280.83 (80)	318 579.78 (53)	
	3G_3	195 601.77 (88)	317 922.54 (80)	
	3F_4	190 882.18 (75)	320 729.86 (84)	
	3F_3	188 981.86 (71)	318 410.96 (78)	
	3F_2	187 504.47 (63)	316 969.98 (79)	
	3D_3	214 501.21 (37)	321 474.77 (82)	
	3D_2	233 127.53 (11)	320 780.54 (61)	
	3D_1	236 054.67 (7)	319 335.84 (54)	
	3P_2	227 225.67 (46)	322 853.87 (46)	
	3P_1	230 452.48 (40)	323 098.77 (35)	
	3P_0	233 150.14 (38)	323 329.24 (84)	
	3S_1	224 955.04 (60)	324 308.75 (36)	
	1G_4	199 445.66 (88)	319 985.71 (50)	
	1F_3	245 392.60 (49)	326 855.84 (76)	
	1D_2	240 860.26 (60)	324 991.75 (65)	
	1P_1	234 300.99 (24)	322 334.26 (35)	
	1S_0	188 549.18 (96)		
	$(^2P)nd$ 3F_4	213 970.69 (76)		
	3F_3	212 694.33 (76)	335 106.00 (71)	
	3F_2	213 459.92 (70)	334 387.56 (78)	
	3D_3	229 160.15 (46)	339 634.17 (56)	
	3D_2	210 720.32 (45)	335 312.70 (43)	
	3D_1	207 138.29 (45)	336 349.15 (63)	
	3P_2	217 113.99 (78)	338 215.16 (56)	
	3P_1	211 855.08 (59)	338 096.04 (64)	
	3P_0	210 509.56 (65)	337 430.25 (81)	
	1F_3	226 491.94 (34)	340 327.91 (64)	
	1D_2	205 272.61 (59)	340 125.52 (35)	
	1P_1	259 133.95 (81)	345 103.6 (70)	

Table VI. Comparison between observed and calculated energy-level values (in cm^{-1}) and calculated percentage compositions for the $4s4p^5 + 4s^24p^3(4d + 5d(+6d) + 5s + 6s(+7s))$ configurations of Rb IV

<i>J</i>	<i>E</i> (obs.)	<i>E</i> (calc.)	Obs.-Calc.	Percentage composition ^a
5	196 977	197 197	− 220	100 (² <i>D</i>)4 <i>d</i> ³ <i>G</i>
	320 662	320 603	58	100 (² <i>D</i>)5 <i>d</i> ³ <i>G</i>
4	171 246	170 815	430	96 (⁴ <i>S</i>)4 <i>d</i> ⁵ <i>D</i>
	190 882	190 578	305	75 (² <i>D</i>)4 <i>d</i> ³ <i>F</i> + 13 (² <i>P</i>)4 <i>d</i> ³ <i>F</i>
	196 281	196 087	194	80 (² <i>D</i>)4 <i>d</i> ³ <i>G</i> + 15 (² <i>D</i>)4 <i>d</i> ³ <i>F</i>
	199 446	199 938	− 492	88 (² <i>D</i>)4 <i>d</i> ³ <i>G</i> + 6 (² <i>D</i>)4 <i>d</i> ³ <i>G</i>
	213 971	213 525	445	76 (² <i>P</i>)4 <i>d</i> ³ <i>F</i> + 9 (² <i>D</i>)4 <i>d</i> ¹ <i>G</i> + 7 (² <i>D</i>)4 <i>d</i> ³ <i>F</i> + 6 (² <i>D</i>)4 <i>d</i> ³ <i>G</i>
	298 877	299 068	− 191	96 (⁴ <i>S</i>)5 <i>d</i> ⁵ <i>D</i>
	318 580	318 327	253	53 (² <i>D</i>)5 <i>d</i> ³ <i>G</i> + 35 (² <i>D</i>)5 <i>d</i> ¹ <i>G</i> + 11 (² <i>P</i>)5 <i>d</i> ³ <i>F</i>
	319 986	320 186	− 200	50 (² <i>D</i>)5 <i>d</i> ¹ <i>G</i> + 34 (² <i>D</i>)5 <i>d</i> ³ <i>G</i> + 16 (² <i>D</i>)5 <i>d</i> ³ <i>F</i>
	320 730	320 566	164	84 (² <i>D</i>)5 <i>d</i> ³ <i>F</i> + 9 (² <i>D</i>)5 <i>d</i> ¹ <i>G</i> + 6 (² <i>D</i>)5 <i>d</i> ³ <i>G</i>
		337 520		85 (² <i>P</i>)5 <i>d</i> ³ <i>F</i> + 7 (² <i>D</i>)5 <i>d</i> ³ <i>G</i> + 6 (² <i>D</i>)5 <i>d</i> ¹ <i>G</i>
3	170 938	170 611	327	95 (⁴ <i>S</i>)4 <i>d</i> ⁵ <i>D</i>
	182 975	183 401	− 426	41 (⁴ <i>S</i>)4 <i>d</i> ⁵ <i>D</i> + 41 (² <i>D</i>)4 <i>d</i> ³ <i>D</i> + 6 (² <i>D</i>)4 <i>d</i> ³ <i>F</i>
	188 982	188 788	194	71 (² <i>D</i>)4 <i>d</i> ³ <i>F</i> + 14 (² <i>P</i>)4 <i>d</i> ³ <i>F</i> + 6 (² <i>D</i>)4 <i>d</i> ³ <i>D</i>
	195 602	195 434	167	88 (² <i>D</i>)4 <i>d</i> ³ <i>G</i> + 7 (² <i>D</i>)4 <i>d</i> ³ <i>F</i>
	212 694	212 557	138	76 (² <i>P</i>)4 <i>d</i> ³ <i>F</i> + 12 (² <i>D</i>)4 <i>d</i> ³ <i>F</i> + 5 (² <i>D</i>)4 <i>d</i> ³ <i>G</i> + 5 (² <i>P</i>)4 <i>d</i> ³ <i>D</i>
	214 501	214 530	− 29	37 (² <i>D</i>)4 <i>d</i> ³ <i>D</i> + 31 (² <i>P</i>)4 <i>d</i> ³ <i>D</i> + 14 (⁴ <i>S</i>)4 <i>d</i> ³ <i>D</i> + 6 (² <i>P</i>)4 <i>d</i> ¹ <i>F</i>
	225 173	225 099	74	64 (⁴ <i>S</i>)5 <i>s</i> ³ <i>D</i> + 16 (² <i>P</i>)4 <i>d</i> ¹ <i>F</i> + 6 (² <i>P</i>)4 <i>d</i> ³ <i>D</i> + 5 (² <i>D</i>)4 <i>d</i> ¹ <i>F</i>
	226 492	227 106	− 615	34 (² <i>P</i>)4 <i>d</i> ¹ <i>F</i> + 33 (² <i>D</i>)4 <i>d</i> ¹ <i>F</i> + 12 (² <i>D</i>)5 <i>s</i> ³ <i>D</i> + 11 (⁴ <i>S</i>)4 <i>d</i> ³ <i>D</i> + 7 (² <i>D</i>)4 <i>d</i> ³ <i>D</i>
	229 160	229 203	− 43	46 (² <i>P</i>)4 <i>d</i> ³ <i>D</i> + 20 (² <i>D</i>)5 <i>s</i> ³ <i>D</i> + 18 (⁴ <i>S</i>)4 <i>d</i> ³ <i>D</i>
	245 393	245 063	330	49 (² <i>D</i>)4 <i>d</i> ¹ <i>F</i> + 36 (² <i>P</i>)4 <i>d</i> ¹ <i>F</i> + 6 (² <i>D</i>)5 <i>d</i> ¹ <i>F</i>
	298 754	298 803	− 49	94 (⁴ <i>S</i>)5 <i>d</i> ⁵ <i>D</i>
	304 526	304 447	79	85 (⁴ <i>S</i>)5 <i>d</i> ³ <i>D</i>
	317 923	317 934	− 12	80 (² <i>D</i>)5 <i>d</i> ³ <i>G</i> + 7 (² <i>P</i>)5 <i>d</i> ³ <i>F</i> + 5 (² <i>D</i>)5 <i>d</i> ³ <i>F</i>
	318 411	318 557	− 146	78 (² <i>D</i>)5 <i>d</i> ³ <i>F</i> + 6 (² <i>D</i>)5 <i>d</i> ³ <i>G</i> + 5 (² <i>D</i>)5 <i>d</i> ³ <i>D</i>
	321 475	321 887	− 413	82 (² <i>D</i>)5 <i>d</i> ³ <i>D</i> + 8 (² <i>D</i>)5 <i>d</i> ³ <i>F</i>
	325 956	326 074	− 119	98 (² <i>D</i>)6 <i>s</i> ³ <i>D</i>
	326 856	327 097	− 241	76 (² <i>D</i>)5 <i>d</i> ¹ <i>F</i> + 5 (² <i>P</i>)5 <i>d</i> ³ <i>D</i>
	335 106	335 165	− 59	71 (² <i>P</i>)5 <i>d</i> ³ <i>F</i> + 19 (² <i>P</i>)5 <i>d</i> ³ <i>D</i> + 6 (² <i>P</i>)5 <i>d</i> ¹ <i>F</i>
	339 634	339 371	263	56 (² <i>P</i>)5 <i>d</i> ³ <i>D</i> + 16 (² <i>P</i>)5 <i>d</i> ¹ <i>F</i> + 8 (² <i>P</i>)5 <i>d</i> ³ <i>F</i> + 6 (² <i>D</i>)5 <i>d</i> ³ <i>F</i>
	340 328	340 336	− 8	64 (² <i>P</i>)5 <i>d</i> ¹ <i>F</i> + 10 (² <i>P</i>)5 <i>d</i> ³ <i>F</i> + 7 (² <i>D</i>)5 <i>d</i> ¹ <i>F</i> + 6 (² <i>D</i>)5 <i>d</i> ³ <i>G</i>
2	134 979	134 891	87	82 (² <i>S</i>) <i>p</i> ⁵ ³ <i>P</i> + 12 (² <i>D</i>)4 <i>d</i> ³ <i>P</i> + 5 (² <i>P</i>)4 <i>d</i> ³ <i>P</i>
	170 888	170 640	248	97 (⁴ <i>S</i>)4 <i>d</i> ⁵ <i>D</i>
	181 481	181 607	− 126	36 (⁴ <i>S</i>)4 <i>d</i> ³ <i>D</i> + 32 (² <i>D</i>)4 <i>d</i> ³ <i>D</i> + 13 (² <i>D</i>)4 <i>d</i> ³ <i>F</i> + 6 (² <i>P</i>)4 <i>d</i> ¹ <i>D</i>
	187 504	187 394	111	63 (² <i>D</i>)4 <i>d</i> ³ <i>F</i> + 14 (² <i>P</i>)4 <i>d</i> ³ <i>F</i> + 12 (² <i>D</i>)4 <i>d</i> ³ <i>D</i> + 9 (⁴ <i>S</i>)4 <i>d</i> ³ <i>D</i>
	203 281	203 357	− 75	96 (⁴ <i>S</i>)5 <i>s</i> ⁵ <i>S</i>
	205 273	204 683	589	59 (² <i>P</i>)4 <i>d</i> ¹ <i>D</i> + 24 (² <i>D</i>)4 <i>d</i> ¹ <i>D</i> + 6 (² <i>P</i>)4 <i>d</i> ³ <i>F</i>
	210 720	210 465	255	45 (² <i>P</i>)4 <i>d</i> ³ <i>D</i> + 29 (² <i>D</i>)4 <i>d</i> ³ <i>D</i> + 15 (⁴ <i>S</i>)4 <i>d</i> ³ <i>D</i>
	213 460	213 493	− 33	70 (² <i>P</i>)4 <i>d</i> ³ <i>F</i> + 21 (² <i>D</i>)4 <i>d</i> ³ <i>F</i>
	217 114	216 996	118	78 (² <i>P</i>)4 <i>d</i> ³ <i>P</i> + 11 (² <i>D</i>)4 <i>d</i> ³ <i>P</i>
	224 044	223 884	161	64 (² <i>D</i>)5 <i>s</i> ³ <i>D</i> + 13 (² <i>P</i>)5 <i>s</i> ³ <i>P</i> + 6 (² <i>D</i>)4 <i>d</i> ³ <i>P</i> + 5 (² <i>D</i>)5 <i>s</i> ¹ <i>D</i>
	227 226	227 670	− 444	46 (² <i>D</i>)4 <i>d</i> ³ <i>P</i> + 24 (² <i>D</i>)5 <i>s</i> ³ <i>D</i> + 10 (² <i>S</i>) <i>p</i> ⁵ ³ <i>P</i> + 8 (² <i>D</i>)5 <i>s</i> ¹ <i>D</i>
	229 046	229 149	− 103	76 (² <i>D</i>)5 <i>s</i> ¹ <i>D</i> + 11 (² <i>D</i>)4 <i>d</i> ³ <i>P</i>
	233 128	233 040	88	38 (² <i>P</i>)4 <i>d</i> ³ <i>D</i> + 24 (⁴ <i>S</i>)4 <i>d</i> ³ <i>D</i> + 11 (² <i>D</i>)4 <i>d</i> ³ <i>D</i> + 7 (² <i>D</i>)4 <i>d</i> ¹ <i>D</i>
	240 860	241 405	− 545	60 (² <i>D</i>)4 <i>d</i> ¹ <i>D</i> + 23 (² <i>P</i>)4 <i>d</i> ¹ <i>D</i> + 7 (² <i>P</i>)4 <i>d</i> ³ <i>D</i>
	243 700	243 402	298	78 (² <i>P</i>)5 <i>s</i> ³ <i>P</i> + 6 (² <i>D</i>)5 <i>s</i> ¹ <i>D</i> + 6 (² <i>D</i>)5 <i>s</i> ³ <i>D</i> + 6 (² <i>D</i>)4 <i>d</i> ³ <i>P</i>
	298 722	298 714	8	95 (⁴ <i>S</i>)5 <i>d</i> ⁵ <i>D</i>
	303 803	303 747	56	81 (⁴ <i>S</i>)5 <i>d</i> ³ <i>D</i>
	304 509	304 449	60	96 (⁴ <i>S</i>)6 <i>s</i> ⁵ <i>S</i>
	316 970	317 260	− 290	79 (² <i>D</i>)5 <i>d</i> ³ <i>F</i> + 6 (² <i>P</i>)5 <i>d</i> ³ <i>F</i>
	320 781	320 943	− 162	61 (² <i>D</i>)5 <i>d</i> ³ <i>D</i> + 19 (² <i>D</i>)5 <i>d</i> ³ <i>P</i> + 6 (² <i>P</i>)5 <i>d</i> ³ <i>P</i>
	322 854	322 721	133	46 (² <i>D</i>)5 <i>d</i> ³ <i>P</i> + 23 (² <i>D</i>)5 <i>d</i> ³ <i>D</i> + 9 (² <i>D</i>)5 <i>d</i> ¹ <i>D</i> + 7 (² <i>D</i>)6 <i>s</i> ³ <i>D</i>
	323 939	323 995	− 57	60 (² <i>D</i>)6 <i>s</i> ³ <i>D</i> + 16 (² <i>D</i>)6 <i>s</i> ¹ <i>D</i> + 10 (² <i>P</i>)6 <i>s</i> ³ <i>P</i> + 8 (² <i>D</i>)5 <i>d</i> ³ <i>P</i>
	324 992	324 766	226	65 (² <i>D</i>)5 <i>d</i> ¹ <i>D</i> + 16 (² <i>D</i>)5 <i>d</i> ³ <i>P</i> + 6 (² <i>D</i>)5 <i>d</i> ³ <i>F</i> + 6 (² <i>P</i>)5 <i>d</i> ¹ <i>D</i>
	326 749	326 861	− 112	74 (² <i>D</i>)6 <i>s</i> ¹ <i>D</i> + 24 (² <i>D</i>)6 <i>s</i> ³ <i>D</i>
	334 388	334 383	4	78 (² <i>P</i>)5 <i>d</i> ³ <i>F</i> + 12 (² <i>P</i>)5 <i>d</i> ¹ <i>D</i>
	335 313	335 374	− 61	43 (² <i>P</i>)5 <i>d</i> ³ <i>D</i> + 30 (² <i>P</i>)5 <i>d</i> ³ <i>P</i> + 22 (² <i>P</i>)5 <i>d</i> ¹ <i>D</i>
	338 215	338 445	− 230	56 (² <i>P</i>)5 <i>d</i> ³ <i>P</i> + 14 (² <i>P</i>)5 <i>d</i> ¹ <i>D</i> + 11 (² <i>P</i>)5 <i>d</i> ³ <i>D</i> + 8 (² <i>D</i>)5 <i>d</i> ³ <i>P</i>
	340 126	340 074	52	35 (² <i>P</i>)5 <i>d</i> ¹ <i>D</i> + 24 (² <i>P</i>)5 <i>d</i> ³ <i>D</i> + 13 (² <i>P</i>)5 <i>d</i> ³ <i>F</i> + 9 (² <i>D</i>)5 <i>d</i> ¹ <i>D</i> + 9 (² <i>D</i>)5 <i>d</i> ³ <i>F</i>
	343 183	343 190	− 8	83 (² <i>P</i>)6 <i>s</i> ³ <i>P</i> + 8 (² <i>D</i>)6 <i>s</i> ³ <i>D</i> + 6 (² <i>D</i>)6 <i>s</i> ¹ <i>D</i>
1	139 618	139 613	5	81 (² <i>S</i>) <i>p</i> ⁵ ³ <i>P</i> + 13 (² <i>D</i>)4 <i>d</i> ³ <i>P</i>
	168 015	167 959	56	52 (² <i>S</i>) <i>p</i> ⁵ ¹ <i>P</i> + 39 (² <i>D</i>)4 <i>d</i> ¹ <i>P</i> + 6 (² <i>P</i>)4 <i>d</i> ¹ <i>P</i>
	170 855	170 654	201	97 (⁴ <i>S</i>)4 <i>d</i> ⁵ <i>D</i>
	183 582	184 294	− 712	50 (⁴ <i>S</i>)4 <i>d</i> ³ <i>D</i> + 44 (² <i>D</i>)4 <i>d</i> ³ <i>D</i>
	207 138	206 775	363	45 (² <i>P</i>)4 <i>d</i> ³ <i>D</i> + 38 (² <i>D</i>)4 <i>d</i> ³ <i>D</i> + 13 (⁴ <i>S</i>)4 <i>d</i> ³ <i>D</i>

Table VI (continued)

<i>J</i>	<i>E</i> (obs.)	<i>E</i> (calc.)	Obs.-Calc.	Percentage composition
	209 942	210 023	— 81	78 (⁴ <i>S</i>)5 <i>s</i> ³ <i>S</i> + 10 (² <i>P</i>)4 <i>d</i> ³ <i>P</i>
	211 855	211 610	245	59 (² <i>P</i>)4 <i>d</i> ³ <i>P</i> + 18 (² <i>D</i>)4 <i>d</i> ³ <i>P</i> + 16 (⁴ <i>S</i>)5 <i>s</i> ³ <i>S</i>
	223 788	223 461	327	54 (² <i>D</i>)5 <i>s</i> ³ <i>D</i> + 27 (² <i>D</i>)4 <i>d</i> ³ <i>S</i> + 5 (² <i>P</i>)5 <i>s</i> ³ <i>P</i>
	224 955	224 578	377	60 (² <i>D</i>)4 <i>d</i> ³ <i>S</i> + 29 (² <i>D</i>)5 <i>s</i> ³ <i>D</i>
	230 452	230 819	— 367	40 (² <i>D</i>)4 <i>d</i> ³ <i>P</i> + 16 (² <i>P</i>)4 <i>d</i> ³ <i>P</i> + 11 (² <i>S</i>) <i>p</i> ⁵ ³ <i>P</i> + 7 (² <i>P</i>)5 <i>s</i> ³ <i>P</i> + 7 (² <i>D</i>)4 <i>d</i> ¹ <i>P</i> + 6 (² <i>S</i>) <i>p</i> ⁵ ¹ <i>P</i>
	234 301	234 398	— 97	24 (² <i>D</i>)4 <i>d</i> ¹ <i>P</i> + 18 (² <i>P</i>)4 <i>d</i> ³ <i>D</i> + 13 (² <i>S</i>) <i>p</i> ⁵ ¹ <i>P</i> + 12 (⁴ <i>S</i>)4 <i>d</i> ³ <i>D</i> + 8 (² <i>P</i>)5 <i>s</i> ³ <i>P</i>
	236 055	236 161	— 106	27 (² <i>P</i>)4 <i>d</i> ³ <i>D</i> + 16 (⁴ <i>S</i>)4 <i>d</i> ³ <i>D</i> + 15 (² <i>D</i>)4 <i>d</i> ¹ <i>P</i> + 13 (² <i>S</i>) <i>p</i> ⁵ ¹ <i>P</i> + 11 (² <i>P</i>)5 <i>s</i> ¹ <i>P</i> + 7 (² <i>D</i>)4 <i>d</i> ³ <i>D</i>
	241 307	241 531	— 224	72 (² <i>P</i>)5 <i>s</i> ³ <i>P</i> + 11 (² <i>D</i>)4 <i>d</i> ³ <i>P</i>
	246 331	246 238	94	72 (² <i>P</i>)5 <i>s</i> ¹ <i>P</i> + 8 (² <i>D</i>)4 <i>d</i> ¹ <i>P</i> + 7 (² <i>D</i>)5 <i>s</i> ³ <i>D</i>
	259 134	258 840	294	81 (² <i>P</i>)4 <i>d</i> ¹ <i>P</i> + 6 (² <i>P</i>)5 <i>d</i> ¹ <i>P</i>
	298 703	298 678	24	96 (⁴ <i>S</i>)5 <i>d</i> ³ <i>D</i>
	304 414	304 367	47	87 (⁴ <i>S</i>)5 <i>d</i> ³ <i>D</i>
	306 728	306 687	41	96 (⁴ <i>S</i>)6 <i>s</i> ³ <i>S</i>
	319 336	319 151	185	54 (² <i>D</i>)5 <i>d</i> ³ <i>D</i> + 27 (² <i>D</i>)5 <i>d</i> ¹ <i>P</i> + 6 (² <i>P</i>)5 <i>d</i> ³ <i>D</i>
	322 334	322 233	102	35 (² <i>D</i>)5 <i>d</i> ¹ <i>P</i> + 29 (² <i>D</i>)5 <i>d</i> ³ <i>S</i> + 19 (² <i>D</i>)5 <i>d</i> ³ <i>D</i> + 7 (² <i>D</i>)5 <i>d</i> ³ <i>P</i> + 6 (² <i>P</i>)5 <i>d</i> ³ <i>P</i>
	323 099	322 910	189	35 (² <i>D</i>)5 <i>d</i> ³ <i>P</i> + 17 (² <i>D</i>)5 <i>d</i> ³ <i>S</i> + 15 (² <i>D</i>)5 <i>d</i> ¹ <i>P</i> + 14 (² <i>D</i>)5 <i>d</i> ³ <i>D</i> + 11 (² <i>D</i>)6 <i>s</i> ³ <i>D</i>
	323 709	323 747	— 38	70 (² <i>D</i>)6 <i>s</i> ³ <i>D</i> + 9 (² <i>D</i>)5 <i>d</i> ³ <i>S</i> + 8 (² <i>D</i>)5 <i>d</i> ¹ <i>P</i> + 5 (² <i>P</i>)6 <i>s</i> ¹ <i>P</i>
	324 309	323 978	331	49 (² <i>D</i>)5 <i>d</i> ³ <i>P</i> + 36 (² <i>D</i>)5 <i>d</i> ³ <i>S</i> + 6 (² <i>D</i>)6 <i>s</i> ³ <i>D</i> + 6 (² <i>D</i>)5 <i>d</i> ¹ <i>P</i>
	336 349	336 050	299	63 (² <i>P</i>)5 <i>d</i> ³ <i>D</i> + 19 (² <i>P</i>)5 <i>d</i> ³ <i>P</i> + 8 (⁴ <i>S</i>)6 <i>d</i> ³ <i>D</i>
	338 096	337 999	97	64 (² <i>P</i>)5 <i>d</i> ³ <i>P</i> + 15 (² <i>P</i>)5 <i>d</i> ³ <i>D</i>
	339 965	339 840	125	74 (² <i>P</i>)6 <i>s</i> ³ <i>P</i> + 22 (² <i>P</i>)6 <i>s</i> ¹ <i>P</i>
	343 853	343 802	51	64 (² <i>P</i>)6 <i>s</i> ¹ <i>P</i> + 18 (² <i>P</i>)6 <i>s</i> ³ <i>P</i> + 12 (² <i>D</i>)6 <i>s</i> ³ <i>D</i>
	345 104	345 494	— 391	70 (² <i>P</i>)5 <i>d</i> ¹ <i>P</i> + 8 (⁴ <i>S</i>)6 <i>d</i> ³ <i>D</i>
0	142 609	142 609	0	82 (² <i>S</i>) <i>p</i> ⁵ ³ <i>P</i> + 13 (² <i>D</i>)4 <i>d</i> ³ <i>P</i>
	170 775	170 579	197	97 (⁴ <i>S</i>)4 <i>d</i> ⁵ <i>D</i>
	188 549	190 297	— 1748	96 (² <i>D</i>)4 <i>d</i> ¹ <i>S</i>
	210 510	210 497	12	65 (² <i>P</i>)4 <i>d</i> ³ <i>P</i> + 29 (² <i>D</i>)4 <i>d</i> ³ <i>P</i>
	233 150	232 974	176	38 (² <i>D</i>)4 <i>d</i> ³ <i>P</i> + 27 (² <i>P</i>)5 <i>s</i> ³ <i>P</i> + 21 (² <i>P</i>)4 <i>d</i> ³ <i>P</i> + 12 (² <i>S</i>) <i>p</i> ⁵ ³ <i>P</i>
	240 818	241 220	— 402	72 (² <i>P</i>)5 <i>s</i> ³ <i>P</i> + 19 (² <i>D</i>)4 <i>d</i> ³ <i>P</i>
	298 684	298 651	33	96 (⁴ <i>S</i>)5 <i>d</i> ⁵ <i>D</i>
		318 934		84 (² <i>D</i>)5 <i>d</i> ¹ <i>S</i>
	323 329	323 387	— 58	84 (² <i>D</i>)5 <i>d</i> ³ <i>P</i> + 10 (² <i>D</i>)5 <i>d</i> ¹ <i>S</i>
	337 430	337 511	— 81	81 (² <i>P</i>)5 <i>d</i> ³ <i>P</i> + 6 (² <i>D</i>)5 <i>d</i> ³ <i>P</i>
		339 568		94 (² <i>P</i>)6 <i>s</i> ³ <i>P</i>

^a Eigenvector components larger than 5% are given.

Mean error of the least-squares fit $\sigma = \left[\frac{\sum (E_{\text{obs}} - E_{\text{calc}})^2}{N - P} \right]^{1/2} = 347 \text{ cm}^{-1}$ with $N = 95$ known levels and $P = 25$ adjustable parameters.

Table VII. Energy parameters (in cm^{-1}) for the $4s4p^5 + 4s^24p^3(4d + 5d + 6d + 5s + 6s + 7s)$ configurations of Rb IV.

Parameter	HF (E_{av})	Fitted	Fitted/HF Rb IV	Fitted/HF Sr V ^a
p^5				
E_{av}		166923 $\pm$ 270		
$G^1(4s, 4p)$	89406	70304 $\pm$ 1030	0.786 $\pm$ 0.012	0.791 $\pm$ 0.011
ξ_{4p}	4871	5320 $\pm$ 390	1.092 $\pm$ 0.080	1.100 $\pm$ 0.066
$5s$				
E_{av}		226731 $\pm$ 140		
$F^2(4p, 4p)$	68300	54467 $\pm$ 790	0.797 $\pm$ 0.012	0.806 $\pm$ 0.013
$G^1(4p, 5s)$	6391	5531 $\pm$ 350	0.865 $\pm$ 0.055	0.881 $\pm$ 0.057
ξ_{4p}	5232	5588 $\pm$ 310	1.068 $\pm$ 0.059	1.142 $\pm$ 0.043
$6s$				
E_{av}		326358 $\pm$ 120		
$F^2(4p, 4p)$	68773	55477 $\pm$ 770	0.807 $\pm$ 0.011	0.814 $\pm$ 0.011
$G^1(4p, 6s)$	1976	1686 $\pm$ 340	0.853 $\pm$ 0.170	0.853 $\pm$ 0.160
ξ_{4p}	5292	6049 $\pm$ 270	1.143 $\pm$ 0.051	1.125 $\pm$ 0.038
$7s$				
E_{av}		370000 (fix)		
$F^2(4p, 4p)$	68882	68882 (fix)	1.0	1.0
$G^1(4p, 7s)$	910	910 (fix)	1.0	1.0
ξ_{4p}	5308	5308 (fix)	1.0	1.0
$4d$				
E_{av}		205738 $\pm$ 66		
$F^2(4p, 4p)$	67290	53833 $\pm$ 470	0.800 $\pm$ 0.007	0.805 $\pm$ 0.008
$F^2(4p, 4d)$	50421	43570 $\pm$ 490	0.864 $\pm$ 0.010	0.874 $\pm$ 0.010
$G^1(4p, 4d)$	60807	51076 $\pm$ 220	0.840 $\pm$ 0.004	0.833 $\pm$ 0.003
$G^3(4p, 4d)$	37288	31172 $\pm$ 620	0.836 $\pm$ 0.017	0.845 $\pm$ 0.017
ξ_{4p}	5054	5970 $\pm$ 180	1.181 $\pm$ 0.036	1.145 $\pm$ 0.029
ξ_{4d}	267	211 $\pm$ 94	0.790 $\pm$ 0.350	0.871 $\pm$ 0.260
$5d$				
E_{av}		321113 $\pm$ 64		
$F^2(4p, 4p)$	68715	56475 $\pm$ 400	0.822 $\pm$ 0.006	0.822 $\pm$ 0.007
$F^2(4p, 5d)$	12748	9778 $\pm$ 890	0.767 $\pm$ 0.070	0.806 $\pm$ 0.069
$G^1(4p, 5d)$	9130	4710 $\pm$ 310	0.516 $\pm$ 0.034	0.596 $\pm$ 0.034
$G^3(4p, 5d)$	6255	1359 $\pm$ 600	0.217 $\pm$ 0.096	0.460 $\pm$ 0.100
ξ_{4p}	5274	6045 $\pm$ 150	1.146 $\pm$ 0.028	1.129 $\pm$ 0.026
ξ_{5d}	76	185 $\pm$ 70	2.434 $\pm$ 0.920	1.661 $\pm$ 0.810
$6d$				
E_{av}		369000 (fix)		
$F^2(4p, 4p)$	68861	68861 (fix)	1.0	1.0
$F^2(4p, 6d)$	5591	5591 (fix)	1.0	1.0
$G^1(4p, 6d)$	11038	11038 (fix)	1.0	1.0
$G^3(4p, 6d)$	3707	3707 (fix)	1.0	1.0
ξ_{4p}	5302	5302 (fix)	1.0	1.0
ξ_{6d}	37	37 (fix)	1.0	1.0
Configuration interaction integrals				
p^5-5s				
$R^1(4p4p, 4s5s)$	2679 (.075) ^b	2679 (fix)	1.0	1.0
p^5-6s				
$R^1(4p4p, 4s6s)$	661 (.031)	661 (fix)	1.0	1.0
p^5-7s				
$R^1(4p4p, 4s7s)$	225 (.015)	225 (fix)	1.0	1.0
p^5-4d				
$R^1(4p4p, 4s4d)$	71813 (.998)	54529 (fix)	0.76	0.76
p^5-5d				
$R^1(4p4p, 4s5d)$	27584 (.890)	20945 (fix)	0.76	0.76
p^5-6d				
$R^1(4p4p, 4s6d)$	17018 (.833)	12922 (fix)	0.76	0.76
$5s-6s$				
$R^1(4p5s, 6s4p)$	3449 (.377)	3449 (fix)	1.0	1.0
$5s-7s$				
$R^1(4p5s, 7s4p)$	2289 (.363)	2289 (fix)	1.0	1.0
$5s-4d$				
$R^2(4p5s, 4p4d)$	— 9197 (— .347)	— 9197 (fix)	1.0	1.0
$R^1(4p5s, 4d4p)$	— 1704 (— .056)	— 1704 (fix)	1.0	1.0

Table VII (continued)

Parameter	HF (E_{av})	Fitted	Fitted/HF Rb IV	Fitted/HF Sr V ^a
5s-5d				
$R^2(4p5s, 4p5d)$	7519 (.614)	7519 (fix)	1.0	1.0
$R^1(4p5s, 5d4p)$	1803 (.144)	1803 (fix)	1.0	1.0
5s-6d				
$R^2(4p5s, 4p6d)$	6012 (.726)	6012 (fix)	1.0	1.0
$R^1(4p5s, 6d4p)$	1606 (.195)	1606 (fix)	1.0	1.0
6s-7s				
$R^1(4p6s, 7s4p)$	1336 (.362)	1336 (fix)	1.0	1.0
6s-4d				
$R^2(4p6s, 4p4d)$	- 4872 (-.322)	- 4872 (fix)	1.0	1.0
$R^1(4p6s, 4d4p)$	- 1648 (-.093)	- 1648 (fix)	1.0	1.0
6s-5d				
$R^2(4p6s, 4p5d)$	- 1142 (-.151)	- 1142 (fix)	1.0	1.0
$R^1(4p6s, 5d4p)$	561 (.076)	561 (fix)	1.0	1.0
6s-6d				
$R^2(4p6s, 4p6d)$	1829 (.389)	1829 (fix)	1.0	1.0
$R^1(4p6s, 6d4p)$	616 (.128)	616 (fix)	1.0	1.0
7s-4d				
$R^2(4p7s, 4p4d)$	- 3292 (-.316)	- 3292 (fix)	1.0	1.0
$R^1(4p7s, 4d4p)$	- 1291 (-.105)	- 1291 (fix)	1.0	1.0
7s-5d				
$R^2(4p7s, 4p5d)$	- 845 (-.165)	- 845 (fix)	1.0	1.0
$R^1(4p7s, 5d4p)$	265 (.052)	265 (fix)	1.0	1.0
7s-6d				
$R^2(4p7s, 4p6d)$	- 167 (-.049)	- 167 (fix)	1.0	1.0
$R^1(4p7s, 6d4p)$	341 (.102)	341 (fix)	1.0	1.0
4d-5d				
$R^2(4p4d, 4p5d)$	15233 (.736)	13557 (fix)	0.89	0.89
$R^1(4p4d, 5d4p)$	22101 (.866)	27847 (fix)	1.26	1.26
$R^3(4p4d, 5d4p)$	14177 (.919)	10916 (fix)	0.77	0.77
4d-6d				
$R^2(4p4d, 4p6d)$	8697 (.643)	7741 (fix)	0.89	0.89
$R^1(4p4d, 6d4p)$	13347 (.799)	16818 (fix)	1.26	1.26
$R^3(4p4d, 6d4p)$	8615 (.862)	6634 (fix)	0.77	0.77
5d-6d				
$R^2(4p5d, 4p6d)$	6937 (.888)	6174 (fix)	0.89	0.89
$R^1(4p5d, 6d4p)$	5716 (.797)	7202 (fix)	1.26	1.26
$R^3(4p5d, 6d4p)$	3985 (.912)	3068 (fix)	0.77	0.77

^a For comparison the ratios between fitted and Hartree-Fock parameter values in Sr V are given in the last column.

^b The values in parentheses are a measure of the amount of cancellation which occurred in forming the integral. These numbers are the ratio of the true R^k value to an R^k value calculated using the absolute value of each wavefunction.

Table VIII. Comparison between observed and calculated energy-level values (in cm^{-1}) and calculated percentage compositions for the $4s^2 4p^3 5p$ configuration of Rb IV

J	$E(\text{obs.})$	$E(\text{calc.})$	Obs.-Calc.	Percentage composition ^a
4	265 237	265 198	38	100 (2D) 3F
3	243 528	243 454	74	96 (4S) 5P
	262 485	262 434	51	66 (2D) 3F + 22 (2D) 3D + 9 (2P) 3D
	264 104	264 141	— 37	52 (2D) 1F + 42 (2D) 3D
	264 885	264 934	— 49	39 (2D) 1F + 36 (2D) 3D + 24 (2D) 3F
	281 835	281 795	40	84 (2P) 3D + 7 (2D) 3F + 6 (2D) 1F
2	242 254	242 198	56	89 (4S) 5P + 6 (4S) 3P
	247 902	247 970	— 68	83 (4S) 3P + 8 (4S) 5P + 6 (2D) 3P
	260 841	260 816	25	45 (2D) 3F + 40 (2D) 3D + 9 (2P) 3D
	262 554	262 490	65	47 (2D) 3D + 42 (2D) 3F + 6 (2P) 1D
	268 186	268 244	— 57	74 (2D) 3P + 10 (2P) 3P + 6 (4S) 3P + 5 (2D) 1D
	274 441	274 335	106	79 (2D) 1D + 9 (2D) 3P
	279 746	279 579	166	79 (2P) 3D + 9 (2P) 3P
	284 487	284 392	95	78 (2P) 1D + 6 (2D) 1D + 6 (2D) 3F
	286 083	286 114	— 31	67 (2P) 3P + 9 (2D) 3P + 7 (2P) 1D + 7 (2D) 1D + 6 (2D) 3D
1	241 924	241 866	58	94 (4S) 5P
	247 061	247 027	34	80 (4S) 3P + 7 (2D) 3P
	258 230	258 415	— 186	42 (2D) 3D + 36 (2D) 1P + 9 (2P) 1P
	262 999	263 217	— 218	47 (2D) 1P + 42 (2D) 3D + 6 (2P) 3D
	269 374	269 406	— 33	75 (2D) 3P + 12 (2P) 3S + 10 (4S) 3P
	277 825	277 776	49	76 (2P) 3D + 15 (2P) 1P
	280 022	279 892	130	77 (2P) 3S + 14 (2D) 3P
	280 676	280 653	23	62 (2P) 3P + 28 (2P) 1P + 5 (2P) 3D
	284 924	285 211	— 287	40 (2P) 1P + 30 (2P) 3P + 9 (2P) 3D + 9 (2D) 3D + 8 (2D) 1P
0	248 171	248 171	1	91 (4S) 3P
	269 251	269 344	— 93	89 (2D) 3P + 7 (2P) 1S
	281 207	281 160	47	94 (2P) 3P
		294 228		90 (2P) 1S + 6 (2D) 3P

^aEigenvector components larger than 5% are given.Mean error of the least-squares fit $\sigma = \left[\frac{\sum (E_{\text{obs}} - E_{\text{calc}})^2}{N - P} \right]^{1/2} = 118 \text{ cm}^{-1}$ with $N = 27$ known levels and $P = 7$ adjustable parameters.Table IX. Energy parameters (in cm^{-1}) for the $4s^2 4p^3 5p$ configuration of Rb IV

Parameter	HF (E_{av})	Fitted	Fitted/HF Rb IV	Fitted/HF Sr V ^a
E_{av}		266151 ± 23		
$F^2(4p, 4p)$	68988	54909 ± 160	0.796 ± 0.002	0.803 ± 0.003
$F^2(4p, 5p)$	17346	16948 ± 230	0.977 ± 0.013	0.977 ± 0.015
$G^0(4p, 5p)$	3352	3373 ± 28	1.006 ± 0.008	1.004 ± 0.008
$G^2(4p, 5p)$	4620	3685 ± 180	0.798 ± 0.039	0.799 ± 0.045
ξ_{4p}	5315	5980 ± 60	1.125 ± 0.011	1.117 ± 0.011
ξ_{5p}	825	1174 ± 53	1.423 ± 0.064	1.364 ± 0.058

^aFor comparison the ratios between fitted and Hartree-Fock parameter values in Sr V are given in the last column.

PAPER III

Revised and extended analysis of Xe III

(Preliminary version)

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Abstract

The spectrum of doubly ionized xenon has been investigated. The study is based on photographic recordings of xenon spectra in the 490 - 6900 Å range. The number of classified lines have been increased from about 300 to about 1400. The lines has been classified as transitions between 73 even levels belonging to the $5s^25p^4$, $5s^25p^36p$, $4f$, $5f$ and $5s^05p^6$ configurations, and 83 odd levels belonging to the $5s5p^5$, $5s^25p^36s$, $7s$, $5d$ and $6d$ configurations. In particular, the identifications include most of the Xe III laser lines. A comparison is made between the results of the present analysis and the published Xe $N_{4,5}^{00}$ Auger spectrum.

1. Introduction

The doubly ionized xenon atom, Xe^{2+} ($Z=54$), is isoelectronic with neutral tellurium. The ground configuration in this sequence is $5s^25p^4$. Though for many years there has been a great demand, from, e.g., laser and collision physics, for improved data on the Xe III spectrum and energy level system very little work has been reported since the 1930's when Boyce [1], Humphreys [2] and Humphreys *et al.* [3] undertook extensive studies of the spectrum. A few reports have appeared treating the lower levels of the spectrum [4,5] and the $5s^05p^6$ 1S_0 level [6].

A large number of strong xenon laser lines were reported already some 20 years ago [7]. Primarily due to the work of the group in La Plata, the laser lines were classified as originating in doubly and trebly ionized xenon, but no further classifications were possible due to the lack of relevant spectroscopic data.

In the present work xenon spectra have been recorded photographically in the 490 - 6900 Å range. When analyzing the vast amount of experimental data extensive use has been made of Hartree-Fock calculations and parametric fits. Configuration-interaction (CI) effects, including Rydberg series CI, have been included in the calculations. The configurations studied are $5s^25p^4$, $5s5p^5$, $5s^05p^6$, $5s^25p^36p$, $6s$, $7s$, $5d$, $6d$ and $4f$. The lowest term of the $5f$ configuration has also been located. The number of classified lines has been increased from about 300 to in all 1400. These lines originate from transitions between 73 even- and 83 odd-parity levels.

The present analysis of the optical Xe III spectrum has consequences for the interpretation of the Auger spectra following ionization in the inner $4d$ subshell of neutral xenon.

2. Experimental

To record the spectrum in the vacuum ultraviolet wavelength range, which was done in Lund, two different light sources were used: a direct current hollow-cathode discharge [8] and a theta-pinch discharge [9]. The spectrum was recorded on a 3 m normal incidence spectrograph with a plate factor in the first diffraction order of 2.77 Å/mm [10]. The wavelength range above 2000 Å was recorded on a 3.4 m Ebert plane grating spectrograph in La Plata. This spectrograph has a plate factor of 5 Å/mm in the first diffraction order. The results of the wavelength measurements in air have been discussed previously [11]. The spectrum was excited in a laser-tube-like source (without end-mirrors) about 1 m in length and with an inner diameter of 3 mm. The tube has inner electrodes and was viewed end-on [12].

The wavelengths and intensities of all classified Xe III lines are given in Table I. In the long-wavelength end of the spectrum, outside the range covered by the present recording, a few lines from an unpublished xenon line-list, kindly put to our disposal by Dr Humphreys have been included. In particular almost all of the reported Xe III laser lines have been classified. The intensity figures are visual estimates of photographic density, but are not on a uniform scale. All the experimentally established Xe III levels are given in Tables II and III.

3. Analysis

Figure 1 shows the relative positions and extensions of the investigated configurations. The levels in $5s^25p^4$, $5s5p^5$ and $5s^05p^6$ are known from previous work [4-6], even if the designation of one level, belonging to the $5s5p^5$ configuration has been revised. The $5s^25p^3n\ell$ configurations can be considered as being built on the ground configuration of Xe IV, $5s^25p^3$, by addition of an outer electron. The parent configuration gives three terms, namely 4S , 2D and 2P . Almost all levels of the $5s^25p^4$, $5s5p^5$, $5s^05p^6$, $5s^25p^36p$, $6s$ and $5d$ configuration have been experimentally established or verified in this work. In the $4f$ configuration 5 of the levels based on the 2P parent term are missing and in the $5s^25p^37s$ and $6d$ configurations only levels based on the 4S and 2D parent terms have been located. In the $5s^25p^35f$ configuration only the levels belonging to the lowest term, $(^4S)^5F$, have been located with certainty.

As can be noticed in figure 1, there are severe overlaps between configurations of the same parity. This leads to heavy mixing of the states belonging to different configurations, even if the matrix elements connecting the states are small. Such mixings occur between $6s$ and $5d$, $7s$ and $6d$ and between $6p$ and $4f$ states.

3.1 Even configurations

When interpreting the observed energy level structure of the even-parity configurations, the total energy matrix for the $5s^25p^4 + 5s^25p^3(6p + 4f + 5f) + 5s5p^5 + 5s^05p^6$ configurations was diagonalised. The calculated and observed energy levels were fitted by least-squares fits, treating some of the energy parameters as free parameters.

As is evident from figure 1, there are large energy separations between the levels of the ground configuration and the excited configurations. In cases like this, it is customary to diagonalize the energy matrix and to perform the least squares fit for the ground configuration separately. However, it was found that a least squares fit to the levels of the ground configuration, omitting the effective interaction parameter, α , gives a large discrepancy between the observed and calculated position of the 1D_2 level. A simple perturbation calculation indicates that, due to a large radial integral ($\sim 67000 \text{ cm}^{-1}$) in the CI matrix element, the interaction between the

s^2p^4 and s^0p^6 configurations gives rise to large shift ($\sim 8000 \text{ cm}^{-1}$) of the 1S_0 level of the ground configuration. In a similar way it is found that the interaction between the ground configuration and a "pure" $5s5p^45d$ configuration give rise to large shifts ($\sim 4000 \text{ cm}^{-1}$) of the 3P and 1D levels, but not to the 1S_0 level. Evidently large specific level shifts may occur from these interactions between distant configurations. It is also found that the $5s^05p^6$ 1S_0 state interacts strongly with the 1S_0 state of the $5s5p^45d$ configuration and substantial mixing of these two states occurs.

To obtain as accurate eigenvector compositions and eigenvalues as possible, and in the light of the above discussion, it was belived to be of importance to include the ground configuration, and the high-lying $5s5p^45d$ configurations in the energy matrix of the even configurations, and to include CI-effects between all the configurations. In fact, it was found that the large specific deviation of the p^4 1D_2 level was removed in this way, even with the configuration interaction parameters fixed at their HF values. As none of the levels belonging to the $5s5p^45d$ configuration has been established experimentally, the energy parameters of this configuration were held fixed at their HF values during the fitting process. (However, the $F^2(5p,5p)$ integral was scaled to 0.8 times the HF value.)

The level structure of the $5s^25p^36p$ and $4f$ configurations are given in figure 2. The position of the observed levels of the lowest term in the $5f$ configuration are also indicated. It should be noted from the figure that $4f$ is almost as low a configuration as $6p$. This reflects the fact that Xe III are close to the lanthanides, and $4f$ is no longer hydrogenic. All levels in the figure are given in LS notation. The designations given generally represents the largest percentage contribution to the eigenvector. However, for many levels the purities are very low, the largest component amounting to only about 30% in some cases. In one case it has even been necessary to use the second largest eigenvector component to name the level. Therefore the LS designations often have very little physical significance.

3.2 Odd configurations

The odd-parity configurations were interpreted, just as the even ones, by means of energy matrix diagonalization and parametric least-squares fits to the energy levels. The energy matrix included the $5s5p^5 + 5s^25p^3(6s+7s+5d+6d)$ configurations.

The detailed structure of $5s5p^5$, $5s^25p^3(5d+6s)$ configurations is shown in figure 3, and the experimentally established part of the $5s^25p^3(6d+7s)$ configurations in figure 4. As can be seen from the figures, there are a number of fortuitous coincidences between $6s$ and $5d$ levels, and between $7s$ and $6d$ levels causing severe mixing of the corresponding states. All levels are given in the LS notation, but, just as for the even-parity levels, these designations often have very little physical significance because of the severe mixing of states

with different L and S . In one case even the third largest eigenvector component was required to name the level.

There is also a heavy mixing between $5s5p^5$ and $5s^25p^35d$ states. This mixing is not caused primarily by close level coincidences, but rather by large matrix elements connecting the states. The mixing is most pronounced for the singlets. There is, in fact, no level having $5s5p^5$ 1P as the largest eigenvector component. On the other hand there are five levels having substantial $5s5p^5$ 1P component in their eigenvectors. As will be discussed below, this mixing of states have some consequences for the possibility of VUV laser actions in Xe^{2+} , as well as on the Auger spectra following ionization of an inner $4d$ electron.

One observation about p^3d configurations, that seems to be quite general, is that the 3S term of the lowest d configuration is predicted far below its observed position. In the $4p^34d$ configuration of Kr III [13], Rb IV [14], Sr V [15], and Y VI [16] the discrepancy is of the order of 3000 cm^{-1} . The discrepancy is present also in lighter elements, for instance in the $2p^33d$ configuration of Ne III [17]. It was shown in refs. 14 and 15 that the discrepancy in the $4p^34d$ configurations of Sr V and Rb IV could to a large extent be accounted for by the introduction of Rydberg series configuration interactions, in particular between $4d$ and $5d$, in the theoretical predictions of the level structure.

In Xe III the deviation between observed and calculated positions of the $5p^35d$ 3S_1 level is 700 cm^{-1} even when using fitted values of the energy parameters. When introducing Rydberg series configuration interaction this deviation decreases to 170 cm^{-1} . At the same time the overall mean error of the fit decreases by approximately 20%. The $5d \leftrightarrow 6d$ R^3 CI integral could not be treated as an adjustable parameter at the same time as the R^1 and R^2 integrals. The R^3 integral was therefore optimized in a series of separate calculations and kept fixed in the final calculation.

In general there are good agreements between the g_J factors calculated and those obtained experimentally by Humphreys *et al.* [3]. However, the observed g_J factors for the two levels with $J=1$, located at 133234 and 138145 cm^{-1} respectively, appears to be too small. For $J=1$, all the possible coupling schemes give $g_J > 0.5$.

4 Discussion

Recently much effort has been devoted to the construction of VUV lasers. One candidate for a VUV laser transition, considered by different groups, is the transition at 1089 Å in Xe^{2+} connecting the odd level at $119\,026\text{ cm}^{-1}$ above the ground state, and the even-parity $5s^05p^6$ 1S_0 state at $210\,857\text{ cm}^{-1}$. The lower state, previously designated as $5s5p^5$ 1P_1 , is considered to decay rapidly to the ground

state while the upper state might be populated by Auger processes. However, as pointed out already, there is a considerable mixing between the $5s5p^5$ and the $5s^25p^35d$ states, and in the present analysis the lower level has been designated $5s^25p^3(^2D)5d\ ^1P_1$. The purity of the state is only 44% and the $5s5p^5\ ^1P_1$ contribution is 28%. The $5s5p^5\ ^1P_1$ state is mixed into a number of different 5d states and this opens many different decay modes for the upper $5s^05p^6\ ^1S_0$ state. This fact probably has to be taken into account when discussing the possibility for laser action on this particular transition. The lifetimes of the $5s5p^5\ ^1P_1$ state has not been calculated, but in the second spectrum of Xe [18] the mixing between the $5s5p^6$ and $5s^25p^3nd$ states leads to destructive interference in the line strengths. The calculated lifetime of the $5s5p^6\ ^2P_{1/2}$ state is found to be orders of magnitude longer than the lifetimes obtained in a single configuration approximation.

The present analysis, in particular as regards the mixing between the $5s5p^5$ and the $5s^25p^35d$ states, has consequences also for the interpretation of the Auger spectrum of xenon following ionization of an 4d electron, the $N_{4,5}00$ spectrum (Figure 5.) This spectrum was recorded and reported on by Werme et al. in 1972 [19], but at that time a detailed analysis was not possible because of the lack of spectroscopic data.

The spectrum consist of lines corresponding to the ion being left in different final states. There are two lines for each final state, corresponding to the fine structure of the initial hole in the 4d shell. One group of strong lines corresponds to the ion being left in the $5s^25p^4$ configuration, another group to the $5s5p^5$ final states and a third group corresponding to the ion being left with an empty 5s shell, i.e., the configuration $5s^05p^6$. The remaining strong lines are satellites and are caused by final state configuration interaction, i.e., in the words of the present study, by the mixing between the $5s5p^5$ and the $5s^25p^35d$ (and possibly 6s) states.

In table VIII a detailed comparison is given between the Auger data and the present optical data. The agreement in energies is very good. It can also be seen that those 5d levels which have a significant $5s5p^5$ contribution to the eigenvector give rise to strong satellite lines in the Auger spectrum.

References

- 1 Boyce, J.C., Phys. Rev. 49, 730 (1936)
- 2 Humphreys, C.J., J. Res. Natl. Bur. Stand., 16, 639 (1936)
- 3 Humphreys, C.J., Meggers, W.F. and deBruin, T.L., J. Res. Natl. Bur. Stand. 23, 683 (1939).
- 4 Hansen, J.E., Persson, W., Physica Scripta 25, 487 (1982).
- 5 Gallardo, M., Massone, C.A. Tagliaferri, A.A., Garavaglia and Persson, W., Physica Scripta 19, 538 (1979).
- 6 Hansen, J.E., Meijer, F.G., Outred, M., Persson, W., and Di Rocco, H.O. Physica Scripta 27, 254 (1983).
- 7 Beck, R., English, W. and Gürs, K., Table of Laser Lines in Gases and Vapours, Springer Berlin, Heidelberg, New York, 1978.
- 8 Persson, W. and Minnhagen, L. Ark. Fys. 37, 273 (1968).
- 9 Pettersson, S.-G., Physica Scripta, 26, 296 (1982).
- 10 Minnhagen, L., Physica Scripta, 11, 38 (1975).
- 11 Reyna Almandos, J.G., Bredice, F., DiRocco, H.O. and Gallardo, M., Opt. Pura Appl. 18, 87 (1985).
- 12 Reyna Almandos, Gallardo, M. and Garavaglia, M., Opt. Pura Appl. 15, 1 (1982).
- 13 Persson, W. Unpublished.
- 14 Persson, W. and Wahlström, C.-G., Physica Scripta 31, 487 (1985).
- 15 Persson, W. and Wahlström, C.-G., Physica Scripta 30, 169 (1984).
- 16 Persson, W. and Reader, J., J. Opt. Soc. B. 3, 959 (1986).
- 17 Persson, W. and DiRocco, O., Work in progress.
- 18 Hansen, J. and Persson, W., To be published.
- 19 Werme, L.O., Bergmark, T. and Siegbahn, K., Physica Scripta 6, 141 (1972).

Figure captions

Figure 1: Gross structure of the observed Xe III configurations.

Figure 2: Structure of the $5s^25p^3(6p+4f)$ configurations of Xe III. The position of the lowest 5f term is also indicated. 6p levels are indicated by fully drawn lines, 4f levels by dashed and 5f levels by broken lines with dots in the center. All levels are given in the LS coupling scheme.

Figure 3: Structure of the $5s5p^5+5s^25p^3(5d+6s)$ configurations of Xe III. $5p^5$ levels are indicated by broken lines with dots in the center, 6s levels by dashed and 5d by fully drawn lines. All levels are given in the LS coupling scheme.

Figure 4: Structure of the $5s^25p^3(6d+7s)$ configurations of Xe III. Only levels based on the 4S and 2D parent terms are experimentally established and indicated in the figure. 6d levels are indicated by fully drawn lines and 7s levels by dashed. All levels are given in the LS coupling scheme.

Figure 5: Xenon $N_{4,5}^{00}$ Auger spectrum, from [19] (With permission from the authors.)

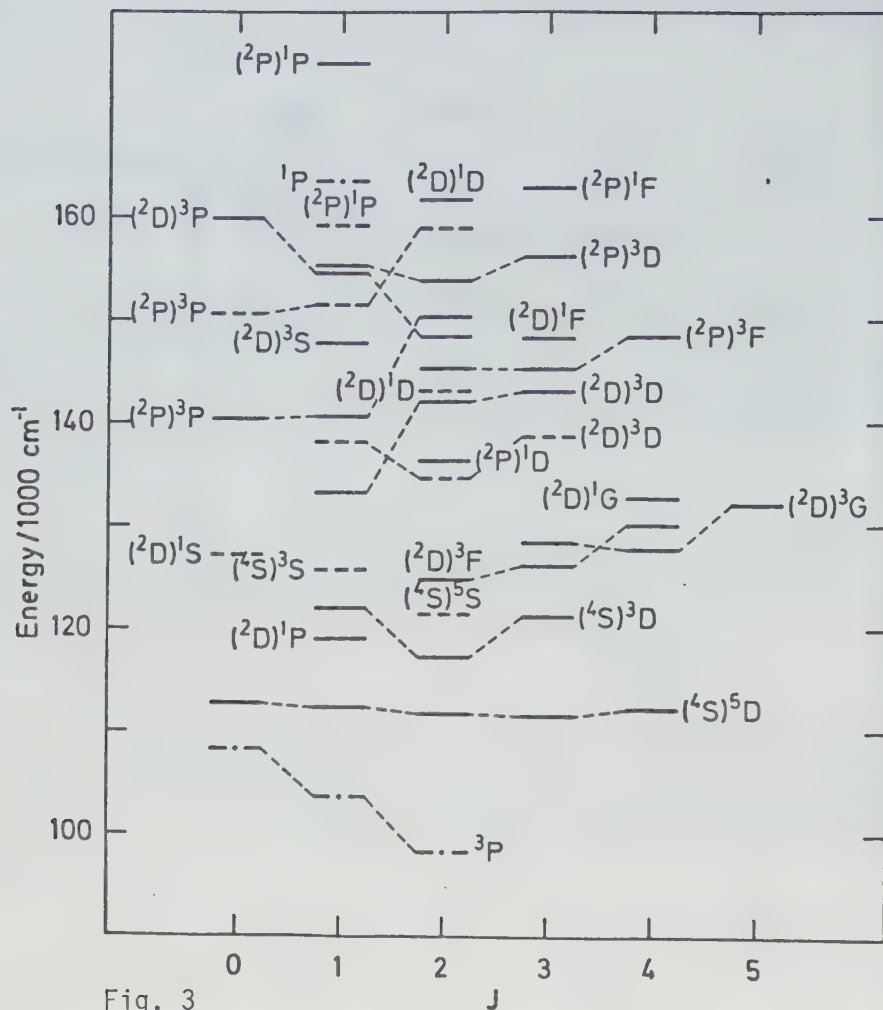


Fig. 3

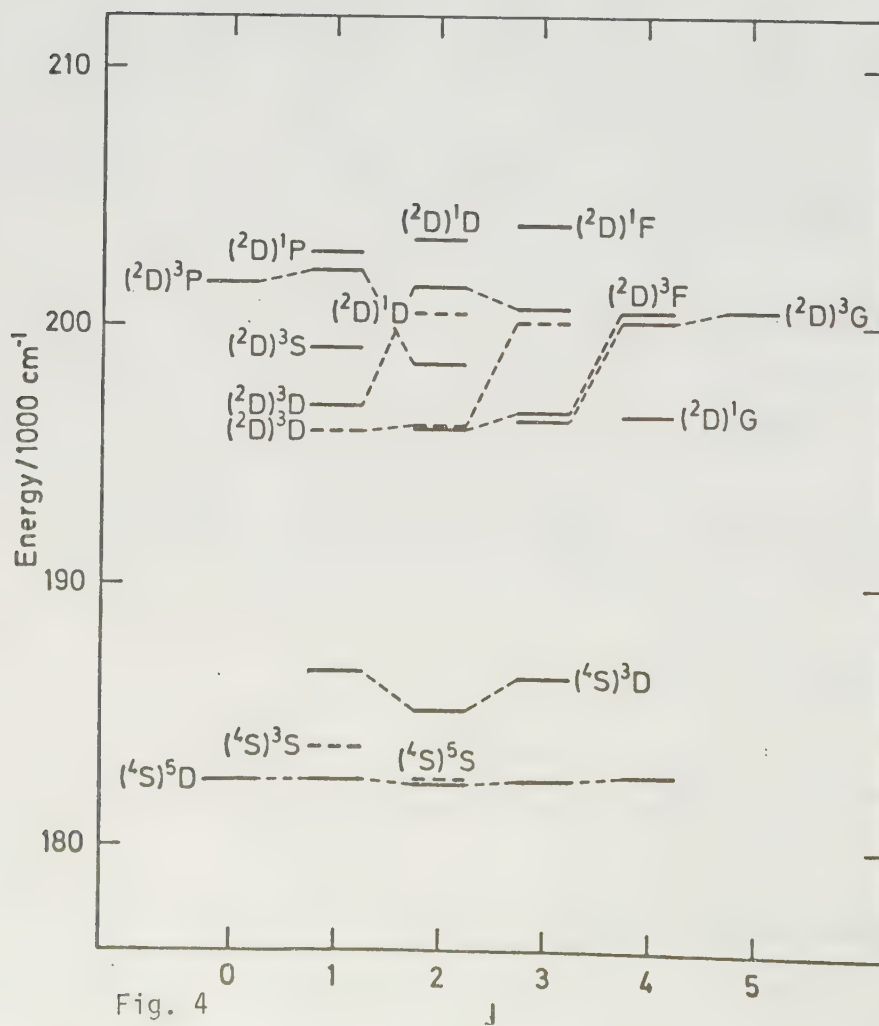


Fig. 4

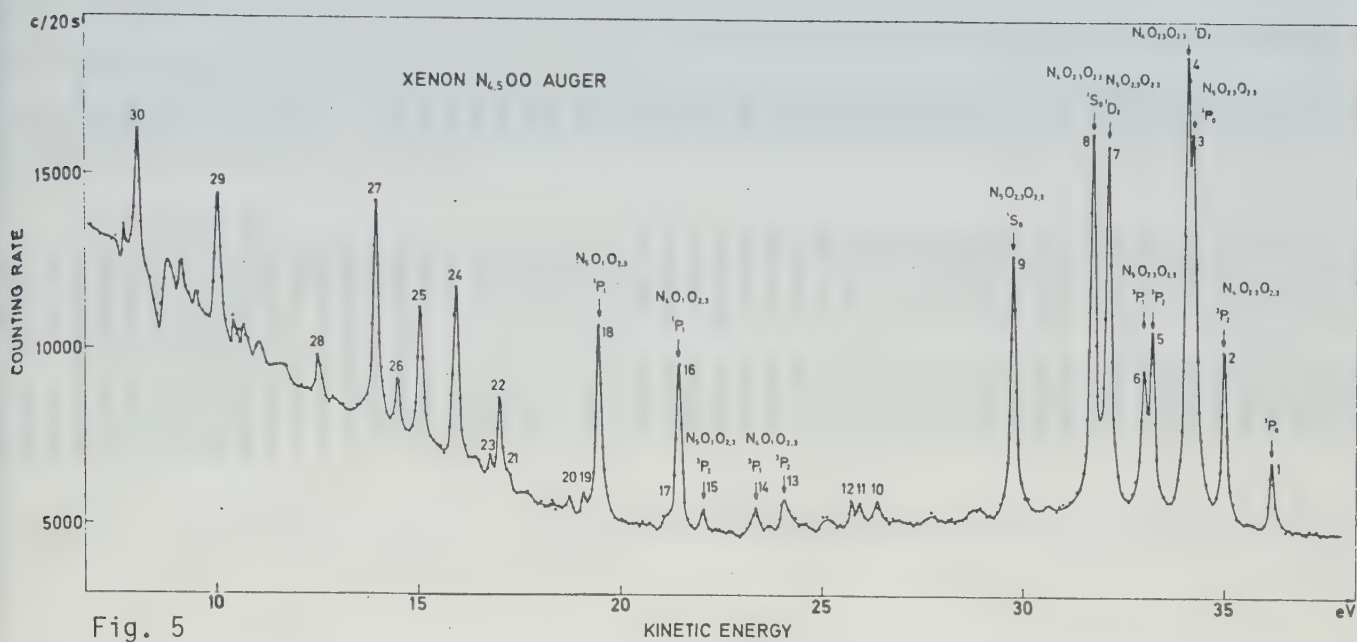


Table I. Observed spectral lines of Xe III. Wavelengths in air are given for lines with $\lambda > 2000 \text{ \AA}$.

Intensity	λ (Å)	obs.	calc.	Classification
2	8869.40	11271.62	(² S)6d ³ D ₁ - (² S)5f ¹ F ₂	
2	8369.894	11944.30	(² P)6p ³ D ₃ - (² D)6d ¹ G ₆	
1	8241.078	12131.00	(² P)6p ¹ D ₂ - (² D)7s ³ D ₂	
2	8239.3	12133.6	(² S)6d ³ D ₃ - (² P)4f ³ F ₂	
20	8047.282	12423.14	(² D)4f ³ G ₅ - (² D)6d ¹ G ₆	
100	8038.262	12437.08	(² S)4f ³ F ₂ - (² S)6d ³ D ₃	
5	8020.07	12465.29	(² S)6d ³ D ₃ - (² S)5f ³ F ₂	
4	7902.902	12650.10	(² S)4f ³ F ₂ - (² S)6d ³ D ₃	
1	7790.5	12832.6	(² S)6d ³ D ₃ - (² P)4f ³ G ₅	
10	7777.116	12854.70	(² S)4f ³ F ₂ - (² S)6d ³ D ₃	
10	7589.397	13172.65	(² P)5d ³ D ₃ - (² P)6p ³ P ₂	
5	7353.025	13596.10	(² D)4f ¹ F ₃ - (² D)6d ¹ D ₂	
10	7311.15	13673.97	(² S)7s ³ S ₂ - (² P)4f ³ F ₂	
100	6949.928	14384.67	(² D)4f ³ H ₆ - (² D)6d ³ G ₅	
0	6895.682	14497.83	(² D)5d ³ P ₀ - (² P)6p ³ D ₁	
0	6858.441	14576.55	(² D)4f ³ H ₆ - (² D)6d ³ G ₅	
2	6850.12	14594.27	(² S)6d ³ D ₃ - (² S)5f ³ F ₂	
0	6847.829	14599.14	(² P)6p ³ D ₂ - (² S)6d ³ D ₃	
0	6815.751	14667.85	(² D)4f ³ F ₂ - (² D)6d ³ G ₅	
1	6799.47	14702.97	(² S)6d ³ D ₃ - (² P)4f ³ F ₂	
4	6780.40	14744.34	(² S)6d ³ D ₃ - (² S)5f ³ F ₂	
0	6767.94	14771.47	(² S)7s ³ S ₂ - (² P)4f ³ F ₂	
0	6759.44	14790.04	(² S)6d ³ D ₃ - (² P)4f ³ F ₂	
3	6733.87	14846.22	(² S)6d ³ D ₃ - (² S)5f ³ F ₂	
1	6722.741	14870.78	(² S)4f ³ F ₂ - (² S)6d ³ D ₃	
1	6698.803	14923.92	(² D)4f ³ H ₆ - (² D)6d ³ F ₃	
1	6665.542	14998.39	(² P)5d ³ F ₃ - (² P)6p ³ D ₂	
0	6657.742	15015.96	(² D)4f ³ F ₂ - (² D)6d ³ F ₃	
3	6656.173	15019.50	(² D)4f ³ P ₁ - (² S)6d ³ P ₂	
1	6638.35	15059.84	(² S)6d ³ D ₃ - (² S)5f ³ F ₂	
1	6625.46	15089.14	(² S)6d ³ D ₃ - (² S)5f ³ F ₂	
1	6622.881	15095.00	(² P)6p ³ D ₂ - (² D)6d ³ S ₁	
3	6619.33	15103.11	(² S)7s ³ S ₂ - (² S)5f ³ F ₂	
2	6611.28	15121.49	(² S)6d ³ D ₃ - (² S)5f ³ F ₂	
0	6608.30	15128.32	(² S)7s ³ S ₂ - (² S)5f ³ F ₂	
0	6585.254	15181.25	(² D)4f ³ H ₆ - (² D)6d ³ G ₅	
1	6556.35	15248.17	(² S)6d ³ D ₃ - (² S)5f ³ F ₂	
1	6541.471	15282.86	(² D)4f ³ F ₂ - (² D)6d ³ D ₁	
1	6530.165	15309.32	(² S)4f ³ F ₁ - (² S)7s ³ S ₂	
1	6530.17	15309.32	(² S)6d ³ D ₃ - (² S)5f ³ F ₂	
1	6513.622	15348.20	(² S)4f ³ F ₁ - (² S)6d ³ D ₁	
1	6513.622	15348.20	(² P)5d ³ F ₁ - (² D)4f ³ G ₅	
0	6501.08	15377.81	(² S)7s ³ S ₂ - (² S)5f ³ F ₂	
0	6501.080	15377.81	(² S)4f ³ F ₁ - (² S)6d ³ D ₁	
0	6493.33	15396.16	(² S)6d ³ D ₃ - (² S)5f ³ F ₂	
1	6484.782	15416.46	(² P)6p ³ P ₂ - (² S)7s ³ S ₂	
1	6462.19	15470.37	(² S)7s ³ S ₂ - (² P)4f ³ G ₅	
1	6456.095	15484.96	(² P)6p ³ P ₂ - (² S)6d ³ D ₁	
0	6454.53	15488.71	(² S)6d ³ D ₃ - (² P)4f ³ G ₅	
0	6409.672	15597.11	(² P)5d ³ D ₃ - (² P)6p ³ D ₂	
0	6407.524	15602.34	(² S)4f ³ F ₂ - (² S)7s ³ S ₂	
2	6396.070	15630.28	(² D)4f ³ P ₁ - (² D)6d ³ S ₁	
5	6367.630	15700.09	(² P)6p ³ P ₁ - (² S)7s ³ S ₁	
1	6341.263	15765.37	(² P)6p ³ D ₃ - (² S)6d ³ D ₃	
0	6333.903	15783.69	(² P)6p ³ D ₃ - (² S)7s ³ S ₂	
1	6283.744	15909.68	(² P)6p ³ F ₂ - (² S)6d ³ D ₃	
0	6275.941	15929.46	(² P)5d ³ F ₃ - (² D)4f ³ G ₅	
1	6273.330	15936.09	(² D)4f ³ G ₅ - (² D)6d ³ G ₆	
0	6268.323	15948.82	(² D)6s ¹ D ₂ - (² P)6p ³ D ₁	
0	6260.092	15969.79	(² P)5d ³ P ₂ - (² S)4f ³ F ₃	
3	6259.041	15972.47	(² S)4f ³ F ₂ - (² S)6d ³ D ₃	
3	6238.181	16025.88	(² D)5d ¹ F ₃ - (² P)6p ¹ F ₃	
2	6221.631	16068.51	(² D)5d ³ P ₂ - (² P)6p ¹ F ₃	
3	6205.954	16109.10	(² S)4f ³ F ₂ - (² S)6d ³ D ₃	
0	6203.813	16114.66	(² S)4f ³ F ₂ - (² S)6d ³ D ₃	
0	6196.423	16133.88	(² S)4f ³ F ₂ - (² S)6d ³ D ₃	
1	6129.094	16311.11	(² D)4f ³ G ₅ - (² D)6d ³ F ₃	
0	6111.902	16356.99	(² P)5d ³ D ₃ - (² S)4f ³ F ₃	
0	6111.772	16357.34	(² D)4f ³ G ₅ - (² D)6d ³ G ₅	
1	6110.352	16361.14	(² S)4f ³ F ₂ - (² S)6d ³ D ₃	
1	6080.350	16496.13	(² D)5d ¹ D ₂ - (² D)4f ³ G ₅	
0	6026.502	16588.78	(² P)5d ³ D ₃ - (² P)6p ¹ D ₂	
1	5969.993	16745.80	(² S)6p ³ P ₁ - 5s ⁵ P ₁	
10	5961.15	16770.64	(² S)6d ³ D ₃ - (² P)4f ³ D ₂	
1	5857.544	17067.27	(² D)4f ³ P ₁ - (² D)7s ¹ D ₂	
1	5857.544	17067.27	(² D)5d ³ D ₃ - (² S)6p ³ P ₁	
0	5780.505	17294.73	(² P)5d ³ F ₂ - (² P)6p ³ F ₃	
0	5761.941	17350.45	(² D)5d ³ P ₁ - (² P)6p ¹ D ₂	
1	5754.022	17374.33	(² D)4f ³ G ₅ - (² D)6d ³ G ₅	
1	5748.671	17390.50	(² D)6s ³ D ₂ - (² S)6p ³ P ₂	
1	5701.233	17535.20	(² D)5d ³ D ₃ - (² P)6p ³ P ₂	
0	5663.842	17650.96	(² D)4f ³ G ₅ - (² D)6d ³ G ₅	
0	5657.234	17671.58	(² D)4f ³ G ₅ - (² D)6d ³ F ₂	
0	5653.871	17682.09	(² P)5d ³ P ₂ - (² P)6p ³ P ₁	
1	5641.253	17721.64	(² D)4f ³ G ₅ - (² D)6d ³ F ₃	
1	5610.181	17819.79	(² P)5d ³ F ₂ - (² S)4f ³ F ₃	
5	5604.331	17838.39	(² P)5d ³ F ₂ - (² S)4f ³ F ₃	
0	5565.831	17961.78	(² D)5d ³ P ₂ - (² S)4f ³ F ₃	
1	5552.773	18004.02	(² D)5d ³ P ₂ - (² S)4f ³ F ₃	
1	5548.043	18019.37	(² P)5d ³ F ₂ - (² P)6p ³ F ₃	
2	5524.326	18096.73	(² P)5d ³ D ₂ - (² P)6p ¹ D ₂	
0	5510.522	18142.06	(² D)5d ¹ F ₃ - (² P)6p ³ F ₃	
0	5509.645	18144.95	(² D)5d ³ S ₁ - (² P)6p ³ P ₀	
0	5503.972	18163.65	(² P)5d ³ F ₂ - (² P)6p ³ D ₃	

0	5481.19	18239.14	'(S)6d	'D ₂ - ('P)4f	'D ₂ - ('P)4f	'D ₂ - ('P)4f	'S ₁ - ('S)6p	'P ₂
0	5470.933	18273.34	'(D)4f	'D ₂ - ('D)6d	'D ₂ - ('D)6d	'D ₂ - ('D)6d	'(P)5d	'D ₂ - ('P)6p
0	5462.121	18302.82	'(D)4f	'G ₃ - ('D)6d	'F ₃	'(D)6s	'D ₂ - ('P)6p	'F ₃
1	5453.055	18333.25	'(P)5d	'D ₁ - ('S)4f	'F ₂	'(P)5d	'F ₂ - ('P)6p	'D ₂
0	5413.492	18467.23	'(D)5d	'P ₁ - ('S)4f	'F ₂	'(D)5d	'P ₁ - ('P)6p	'S ₁
1	5401.004	18509.93	'(D)5d	'P ₂ - ('S)4f	'F ₂	'(D)6s	'D ₂ - ('P)6p	'P ₁
1	5386.634	18559.31	'(P)5d	'P ₁ - ('P)6p	'D ₁	'(D)4f	'D ₂ - ('D)6d	'F ₃
0	5384.144	18567.89	'(P)6s	'P ₁ - ('P)6p	'D ₂	'(P)6p	'D ₂ - ('S)7s	'S ₁
1	5372.825	18607.01	5s 5p ³	'P ₁ - ('P)6p	'S ₁	'(P)5d	'P ₁ - ('P)6p	'D ₂
1	5371.003	18613.32	'(D)5d	'G ₃ - ('S)6p	'P ₂	'(P)5d	'F ₃ - ('S)4f	'F ₂
0	5367.033	18627.09	'(D)5d	'D ₂ - ('P)6p	'F ₂	'(P)5d	'F ₂ - ('S)4f	'F ₂
0	5364.383	18636.29	'(P)5d	'F ₃ - ('D)4f	'F ₂	'(D)4f	'G ₃ - ('D)6d	'G ₃
1	5347.871	18693.83	'(D)4f	'H ₃ - ('D)6d	'G ₃	'(P)5d	'F ₃ - ('P)6p	'D ₂
1	5347.173	18696.27	'(D)5d	'P ₂ - ('P)6p	'P ₂	'(D)5d	'D ₂ - ('D)4f	'P ₁
0	5322.794	18781.90	'(P)6p	'D ₂ - ('D)6d	'D ₂	'(P)5d	'F ₃ - ('P)6p	'P ₂
0	5310.966	18823.73	'(D)5d	'D ₁ - ('S)6p	'P ₂	'(D)5d	'F ₃ - ('S)4f	'F ₃
1	5292.914	18887.93	'(D)5d	'F ₃ - ('S)6p	'P ₃	'(D)5d	'P ₂ - ('S)4f	'F ₃
0	5242.665	19068.96	'(D)4f	'H ₃ - ('D)6d	'F ₃	'(P)6p	'P ₂ - ('S)6d	'D ₁
2	5238.923	19082.58	'(D)5d	'S ₁ - ('S)4f	'F ₂	'(D)6s	'D ₂ - ('D)7s	'D ₂
0	5233.953	19100.70	'(P)6s	'P ₂ - ('P)6p	'P ₁	'(D)6s	'D ₂ - ('P)6p	'F ₂
1	5233.101	19103.81	'(D)5d	'D ₂ - ('P)6p	'D ₂	'(P)6p	'P ₁ - ('S)6d	'D ₁
0	5229.991	19115.17	'(D)4f	'H ₃ - ('D)6d	'G ₃	'(P)6p	'D ₂ - ('D)7s	'D ₂
1	5223.613	19138.51	'(P)5d	'F ₂ - ('P)6p	'F ₃	'(D)5d	'F ₃ - ('S)6p	'P ₁
0	5203.664	19211.88	'(D)6s	'D ₂ - ('P)6p	'D ₂	'(D)5d	'D ₂ - ('P)6p	'D ₂
0	5148.032	19419.49	'(P)5d	'F ₃ - ('D)4f	'D ₃	'(P)5d	'P ₁ - ('P)4f	'F ₂
1	5142.973	19438.59	'(D)5d	'D ₂ - ('P)6p	'F ₃	'(D)4f	'F ₂ - ('D)6d	'F ₃
0	5114.523	19546.72	'(D)6s	'D ₂ - ('P)6p	'P ₃	'(P)6s	'P ₁ - ('S)4f	'F ₂
1	5107.332	19574.24	'(D)5d	'D ₁ - ('S)6p	'P ₁	'(D)5d	'F ₂ - ('S)6p	'P ₂
1	5041.395	19830.25	'(P)5d	'D ₁ - ('P)6p	'D ₁	'(S)4f	'F ₃ - ('D)6d	'G ₃
0	5040.056	19835.52	'(P)6p	'D ₂ - ('D)6d	'F ₃	5s 5p ³	'P ₁ - ('P)6p	'P ₁
1	5038.613	19841.20	'(P)5d	'D ₂ - ('S)4f	'F ₂	'(D)5d	'D ₂ - ('P)6p	'F ₃
1	5023.005	19902.85	'(D)4f	'P ₁ - ('D)6d	'D ₂	'(D)5d	'D ₂ - ('P)6p	'P ₁
0	5008.523	19960.40	'(P)5d	'P ₁ - ('P)6p	'F ₂	'(D)6s	'D ₁ - ('P)6p	'F ₂
0	4996.103	20010.02	'(S)4f	'F ₃ - ('S)6d	'D ₃	'(P)5d	'D ₁ - ('P)6p	'P ₁
0	4952.532	20186.06	'(D)4f	'G ₃ - ('D)6d	'P ₂	'(P)5d	'D ₁ - ('P)6p	'P ₁
1	4927.513	20288.55	'(D)5d	'S ₁ - ('P)6p	'P ₁	'(P)6s	'P ₁ - ('P)6p	'S ₁
0	4926.716	20291.83	'(P)6p	'D ₂ - ('S)6d	'D ₁	'(P)5d	'D ₂ - ('P)6p	'D ₂
0	4918.865	20324.22	'(D)5d	'D ₂ - ('P)6p	'S ₁	5s 5p ³	'P ₁ - ('P)6p	'P ₂
1	4881.044	20481.70	'(D)5d	'P ₁ - ('P)6p	'D ₂	'(P)5d	'F ₂ - ('P)6p	'P ₁
3	4869.404	20530.66	'(D)5d	'D ₂ - ('P)6p	'F ₃	'(P)5d	'F ₂ - ('P)6p	'P ₁
3	4796.504	20842.69	'(D)5d	'F ₃ - ('S)6p	'P ₂	5s 5p ³	'P ₁ - ('P)6p	'P ₂
5	4794.492	20851.44	'(D)6s	'D ₁ - ('P)6p	'D ₁	'(P)6p	'D ₂ - ('S)6d	'D ₂
2	4781.082	20909.92	'(P)6p	'D ₁ - ('D)7s	'D ₂	'(D)5d	'F ₃ - ('S)6p	'P ₃
5	4757.314	21014.39	'(P)5d	'F ₃ - ('S)4f	'F ₃	'(S)4f	'F ₂ - ('D)6d	'D ₁
2	4753.082	21033.10	'(P)5d	'P ₂ - ('S)4f	'F ₃	'(D)5d	'D ₂ - ('S)4f	'F ₃
5	4748.934	21051.47	'(P)5d	'F ₃ - ('P)6p	'D ₂	'(P)6s	'P ₂ - ('P)6p	'S ₁
5	4743.895	21073.83	'(P)5d	'F ₂ - ('S)4f	'F ₃	'(D)4f	'G ₃ - ('D)6d	'D ₂
5	4723.594	21164.40	'(S)6s	'S ₁ - ('S)6p	'P ₁	'(D)5d	'D ₂ - ('S)4f	'F ₃
2	4712.574	21213.89	'(P)5d	'F ₃ - ('P)6p	'F ₃	'(P)6p	'D ₁ - ('D)6d	'P ₂
1	4697.415	21282.35	'(D)5d	'D ₂ - ('P)6p	'F ₃	'(D)6s	'D ₂ - ('S)4f	'F ₃
2	4685.132	21337.87	'(P)5d	'D ₂ - ('P)6p	'D ₁	'(D)6s	'D ₂ - ('S)4f	'F ₃

0	4278.903	23363.90	(² P)5d	¹ F ₃ - (² P)6p	³ P ₁	0	3932.806	25419.94	(² P)6p	³ D ₁ - (² D)6d	¹ D ₁
0	4274.134	23389.97	(² D)5d	³ P ₁ - (² P)6p	³ P ₁	5	3922.546	25486.43	(² S)6s	³ S ₂ - (² S)6p	³ P ₂
4	4272.576	23398.50	(² D)5d	³ D ₃ - (² P)6p	³ F ₄	2	3915.307	25533.55	(² D)5d	¹ F ₃ - (² S)4f	³ F ₄
3	4263.396	23448.88	(² P)6s	³ P ₂ - (² D)4f	³ D ₁	2	3903.666	25609.69	(² D)5d	³ F ₃ - (² S)6p	³ P ₁
0	4246.377	23542.86	(² D)5d	³ D ₃ - (² P)6p	³ D ₁	4	3895.047	25666.36	(² P)6s	³ P ₂ - (² P)6p	³ D ₃
4	4240.235	23576.96	(² D)5d	¹ F ₃ - (² P)6p	³ D ₁	0	3890.976	25693.21	(² P)6p	³ F ₂ - (² S)6d	³ D ₃
2	4235.754	23601.90	(² D)6s	³ D ₃ - (² P)6p	³ D ₂	2	3884.987	25732.82	(² S)5d	³ D ₃ - (² S)6p	³ P ₂
2	4226.966	23650.97	(² D)6s	³ D ₃ - (² P)6p	³ D ₃	4	3880.457	25762.86	(² D)5d	³ D ₁ - (² P)6p	³ D ₁
2	4216.703	23708.53	(² D)5d	³ G ₃ - (² S)6p	³ P ₂	5	3877.817	25780.40	(² D)6s	³ D ₃ - (² P)6p	¹ F ₃
4	4213.986	23723.82	(² D)5d	³ D ₃ - (² S)4f	³ F ₂	1	3861.506	25889.29	(² P)6p	³ D ₂ - (² D)6d	¹ F ₃
3	4209.583	23748.63	(² P)6s	³ P ₁ - (² P)6p	³ D ₁	3	3861.036	25892.44	(² P)5d	³ D ₂ - (² P)6p	³ D ₂
2	4203.883	23780.83	(² P)5d	³ P ₁ - (² P)6p	³ P ₁	1	3860.187	25898.14	(² P)6p	³ F ₂ - (² S)6d	³ D ₁
0	4202.383	23789.32	(² P)6p	³ F ₃ - (² S)6d	³ D ₃	3	3854.277	25937.85	(² D)5d	³ F ₃ - (² S)6p	³ P ₂
2	4195.704	23827.19	(² D)4f	³ D ₂ - (² P)6d	³ D ₁	1	3847.397	25984.23	(² P)5d	³ D ₃ - (² D)4f	³ D ₃
2	4194.864	23831.96	(² D)6s	³ D ₂ - (² S)4f	³ F ₂	3	3841.867	26021.63	(² D)5d	³ D ₂ - (² P)6p	³ P ₁
1	4181.146	23910.15	(² D)5d	³ D ₃ - (² P)6p	³ P ₂	4	3841.526	26023.94	(² D)6s	³ D ₂ - (² P)6p	³ F ₂
5	4176.524	23936.61	(² D)6s	³ D ₃ - (² P)6p	³ F ₂	1	3829.706	26104.26	(² S)4f	³ F ₄ - (² D)6d	³ G ₄
0	4167.595	23987.89	(² P)6p	³ D ₂ - (² D)6d	³ F ₂	0	3823.146	26149.05	(² P)5d	³ P ₁ - (² S)4f	³ F ₂
1	4162.364	24018.04	(² D)6s	³ D ₂ - (² P)6p	³ P ₂	0	3819.487	26174.10	5s 5p ³	¹ P ₁ - (² D)4f	³ P ₁
1	4154.654	24062.61	(² P)5d	³ D ₃ - (² P)6p	³ D ₂	1	3816.776	26192.69	(² P)5d	³ D ₁ - (² D)4f	³ F ₂
1	4152.735	24073.73	(² P)5d	³ P ₀ - (² P)6p	³ P ₁	0	3811.736	26227.32	(² P)5d	³ D ₂ - (² P)6p	³ F ₃
3	4152.036	24077.78	(² D)5d	³ D ₂ - (² P)6p	³ P ₁	1	3802.976	26287.73	(² S)4f	³ F ₃ - (² D)6d	¹ G ₄
0	4150.774	24085.10	(² P)6s	³ P ₁ - (² D)4f	³ P ₁	2	3801.707	26296.51	5s 5p ³	¹ P ₁ - (² D)4f	¹ D ₂
4	4145.743	24114.33	(² D)6s	³ D ₁ - (² P)6p	³ D ₂	0	3792.737	26358.70	(² S)4f	³ F ₃ - (² D)6d	³ F ₃
1	4143.923	24124.92	(² D)6s	³ D ₂ - (² S)4f	³ F ₁	3	3791.667	26366.14	(² D)6s	³ D ₁ - (² P)6p	¹ P ₁
3	4141.993	24136.16	(² P)5d	³ D ₂ - (² P)6p	³ P ₁	5	3780.997	26440.54	(² S)6s	³ S ₁ - (² S)6p	³ P ₂
2	4132.396	24192.21	(² D)5d	³ S ₁ - (² P)6p	³ D ₁	5	3776.317	26473.31	(² P)6s	³ P ₁ - (² P)6p	³ D ₂
0	4112.422	24309.71	(² D)5d	³ D ₂ - (² S)4f	³ F ₂	0	3775.487	26479.13	(² S)4f	³ F ₄ - (² D)6d	³ F ₄
2	4110.043	24323.78	(² P)5d	³ D ₂ - (² P)6p	³ F ₂	4	3772.526	26499.91	(² P)6s	³ P ₁ - (² P)6p	¹ P ₁
4	4109.075	24329.51	(² D)6s	³ D ₂ - (² P)6p	³ D ₁	0	3772.247	26501.87	(² P)6p	³ D ₂ - (² D)6d	³ P ₂
0	4095.026	24412.98	(² P)5d	³ D ₂ - (² D)4f	³ G ₃	2	3768.926	26525.22	(² S)4f	³ F ₄ - (² D)6d	³ G ₃
0	4080.745	24498.41	(² P)6p	³ P ₂ - (² P)6d	³ D ₁	4	3765.847	26546.91	(² P)6s	³ P ₁ - (² P)6p	³ P ₁
2	4078.696	24510.72	(² D)5d	³ D ₂ - (² P)6p	³ P ₂	4	3762.277	26572.10	(² P)6s	³ P ₁ - (² P)6p	³ P ₀
0	4072.966	24545.20	(² P)6s	³ P ₂ - (² D)4f	³ P ₁	1	3757.976	26602.51	(² D)5d	³ D ₂ - (² D)4f	³ P ₂
4	4060.446	24620.88	(² P)6s	³ P ₁ - (² P)6p	³ D ₂	1	3751.437	26648.88	(² P)5d	³ F ₃ - (² P)6p	¹ D ₂
2	4058.145	24634.84	(² D)5d	³ D ₂ - (² P)6p	³ D ₃	5	3745.706	26689.65	(² P)5d	³ F ₂ - (² P)6p	¹ D ₂
5	4050.066	24683.98	(² S)6s	³ S ₁ - (² S)6p	³ P ₁	0	3743.737	26703.69	(² S)4f	³ F ₄ - (² D)6d	³ D ₃
3	4043.226	24725.74	(² P)6s	³ P ₀ - (² P)6p	³ D ₁	0	3739.597	26733.25	(² P)5d	³ D ₁ - (² P)6p	³ S ₁
1	4032.906	24789.01	(² P)6p	³ D ₁ - (² S)7s	³ S ₁	1	3728.906	26809.89	(² P)6p	³ D ₂ - (² P)6d	³ D ₁
2	4028.556	24815.78	(² D)5d	³ D ₂ - (² S)4f	³ F ₂	0	3721.817	26860.96	(² D)5d	³ P ₂ - (² P)6p	³ D ₁
0	4026.816	24826.50	(² P)5d	³ P ₂ - (² P)6p	³ D ₁	0	3721.027	26866.66	(² P)5d	³ F ₃ - (² D)4f	¹ D ₂
2	4021.597	24858.72	(² S)5d	³ D ₁ - (² S)6p	³ P ₁	2	3711.907	26932.67	(² P)6s	³ P ₁ - (² P)6p	³ P ₂
1	3998.546	25002.02	(² D)5d	³ D ₂ - (² P)6p	³ P ₂	3	3708.936	26954.24	(² D)5d	³ P ₁ - (² D)4f	³ F ₂
4	3992.846	25037.71	(² D)6s	³ D ₁ - (² P)6p	³ P ₁	3	3708.147	26959.98	(² P)6s	³ P ₂ - (² P)6p	¹ P ₁
1	3992.537	25039.65	(² S)5d	³ D ₁ - (² S)6p	³ P ₂	1	3707.627	26963.76	5s 5p ³	¹ P ₁ - (² P)6p	¹ S ₀
3	3985.956	25080.99	(² P)6s	³ P ₂ - (² P)6p	¹ D ₂	1	3689.827	27093.83	(² D)5d	³ D ₃ - (² S)4f	³ F ₃
2	3969.906	25182.39	(² D)5d	³ D ₂ - (² D)4f	³ D ₂	1	3687.037	27114.33	(² P)6p	³ D ₂ - (² D)6d	³ S ₁
2	3965.446	25210.71	(² P)5d	³ P ₁ - (² P)6p	³ P ₀	5	3676.627	27191.10	(² S)6s	³ S ₁ - (² S)6p	³ P ₀
5	3950.586	25305.54	(² S)6s	³ S ₂ - (² S)6p	³ P ₁	0	3675.167	27201.90	(² D)6s	³ D ₂ - (² S)4f	³ F ₃
0	3950.116	25308.55	(² P)6p	³ D ₁ - (² D)7s	¹ D ₂	3	3654.607	27354.93	(² P)5d	³ P ₁ - (² P)6p	³ P ₁
0	3941.496	25363.90	(² D)5d	³ P ₂ - (² S)4f	³ F ₂	2	3653.087	27366.31	(² D)5d	³ F ₂ - (² S)6p	³ P ₂

2	3649.566	27392.71	(² P)6s	³ P ₂ - (² P)6p	³ P ₂	4	3467.217	28833.32	(² D)5d	³ D ₃ - (² P)6p	¹ D ₂
2	3644.137	27433.52	(² D)5d	³ S ₁ - (² P)6p	³ D ₁	5	3454.267	28941.41	(² D)6s	¹ D ₂ - (² P)6p	¹ D ₂
3	3640.986	27457.26	(² D)5d	³ D ₁ - (² P)6p	³ F ₂	1	3451.227	28966.90	(² S)4f	³ F ₁ - (² D)7s	³ D ₂
2	3636.016	27494.79	(² D)5d	³ P ₀ - (² P)6p	³ S ₁	1	3451.227	28966.90	(² D)5d	³ P ₀ - (² D)4f	³ P ₁
4	3632.136	27524.16	(² P)6s	³ P ₀ - (² P)6p	³ P ₁	4	3444.386	29024.43	(² P)6s	³ P ₁ - (² D)4f	³ P ₂
1	3628.516	27551.62	(² P)5d	³ P ₂ - (² P)6p	³ D ₂	4	3444.237	29025.69	(² D)5d	³ D ₁ - (² P)6p	³ D ₂
5	3624.057	27585.52	(² S)6s	³ S ₂ - (² S)6p	³ P ₃	3	3435.737	29097.50	(² S)4f	³ F ₂ - (² D)6d	³ F ₂
5	3623.127	27592.60	(² D)6s	³ D ₂ - (² P)6p	³ D ₃	1	3414.537	29278.15	(² P)6p	³ D ₃ - (² D)6d	³ F ₂
1	3621.586	27604.34	(² P)6s	³ P ₁ - (² D)4f	³ D ₂	2	3403.907	29369.58	(² D)5d	³ P ₁ - (² P)6p	¹ D ₂
2	3619.997	27616.46	(² P)5d	³ D ₃ - (² P)6p	³ D ₂	1	3399.867	29404.48	(² P)6s	³ P ₁ - (² D)4f	¹ D ₁
2	3618.857	27625.16	(² P)5d	³ P ₂ - (² P)6p	³ P ₁	0	3395.527	29442.06	(² P)6p	³ D ₃ - (² D)7s	¹ D ₂
2	3615.857	27648.08	(² P)5d	³ P ₀ - (² P)6p	³ P ₁	2	3390.637	29484.52	(² P)6s	³ P ₂ - (² D)4f	¹ P ₂
4	3609.457	27697.10	(² D)6s	³ D ₃ - (² S)4f	³ F ₂	0	3386.227	29522.92	(² P)6p	³ D ₃ - (² D)6d	³ D ₂
1	3609.067	27700.09	(² P)5d	³ D ₂ - (² D)4f	³ F ₂	2	3384.097	29541.50	(² S)5d	³ D ₂ - (² S)6p	³ P ₁
4	3607.016	27715.84	(² D)6s	³ D ₃ - (² S)4f	³ F ₂	2	3383.917	29543.07	(² P)6p	³ P ₂ - (² D)6d	³ F ₃
2	3601.867	27755.46	(² D)5d	³ D ₁ - (² S)6p	³ P ₁	2	3383.917	29543.07	(² D)5d	³ F ₃ - (² P)6p	³ D ₂
4	3596.587	27796.21	(² P)6s	³ D ₁ - (² P)6p	³ P ₀	1	3381.637	29562.99	(² P)6p	³ D ₃ - (² D)6d	³ G ₃
1	3593.377	27821.04	(² P)6p	³ P ₁ - (² D)7s	³ D ₁	1	3379.027	29585.82	(² D)5d	³ P ₂ - (² P)6p	³ D ₂
3	3591.977	27831.88	(² S)5d	³ D ₃ - (² S)6p	³ P ₃	0	3376.977	29603.78	(² S)4f	³ F ₃ - (² D)6d	³ F ₂
1	3584.267	27891.75	(² P)6p	³ P ₁ - (² D)6d	³ F ₂	1	3370.646	29659.38	(² D)5d	³ P ₂ - (² P)6p	³ P ₁
1	3584.267	27891.75	(² D)5d	³ D ₂ - (² D)4f	³ P ₁	1	3365.696	29703.00	(² S)4f	³ F ₁ - (² D)6d	³ D ₁
5	3583.647	27896.57	(² D)6s	³ D ₃ - (² P)6p	³ F ₂	1	3363.317	29706.35	(² P)6p	³ F ₂ - (² D)6d	³ G ₃
5	3579.696	27927.36	(² D)6s	³ D ₂ - (² P)6p	³ F ₂	0	3363.497	29722.42	(² S)5d	³ D ₂ - (² S)6p	³ P ₂
1	3578.536	27936.41	(² D)5d	³ P ₁ - (² S)6p	³ P ₂	1	3362.767	29728.87	(² S)4f	³ F ₂ - (² D)6d	³ F ₃
1	3574.397	27968.76	(² D)5d	³ D ₂ - (² D)4f	¹ F ₃	0	3358.497	29766.67	(² S)4f	³ F ₃ - (² D)7s	³ D ₂
0	3568.627	28013.98	(² D)5d	³ D ₂ - (² D)4f	¹ D ₂	3	3357.987	29771.19	(² D)6s	³ D ₂ - (² P)6p	¹ F ₃
4	3565.187	28041.01	(² D)6s	³ D ₃ - (² P)6p	³ D ₃	1	3353.536	29810.70	(² P)6p	³ P ₂ - (² D)6d	¹ D ₁
1	3564.857	28043.61	(² P)6p	³ D ₂ - (² D)7s	³ D ₃	1	3350.347	29839.08	(² P)6p	³ D ₃ - (² D)6d	¹ G ₃
2	3562.986	28058.33	(² D)5d	³ P ₀ - (² D)4f	³ D ₁	2	3349.757	29844.33	(² D)6s	³ D ₂ - (² P)6p	¹ P ₁
3	3562.217	28064.39	(² P)6s	³ P ₂ - (² D)4f	³ D ₂	4	3345.487	29882.42	(² D)5d	³ G ₃ - (² P)6p	³ F ₃
3	3561.367	28071.09	(² P)5d	³ D ₂ - (² P)6p	¹ F ₃	1	3344.927	29887.43	(² S)4f	³ F ₃ - (² D)6d	³ G ₃
1	3561.227	28072.19	(² P)5d	³ D ₁ - (² D)4f	¹ P ₁	0	3344.267	29893.32	(² D)5d	³ F ₃ - (² D)4f	³ G ₃
4	3552.116	28144.19	(² P)5d	³ D ₂ - (² P)6p	¹ P ₁	3	3340.667	29925.54	(² D)5d	³ D ₂ - (² P)6p	¹ D ₁
1	3546.876	28185.77	(² D)5d	³ D ₂ - (² S)4f	³ D ₃	3	3340.366	29928.23	(² P)5d	³ D ₃ - (² P)6p	³ P ₂
2	3544.856	28201.83	(² P)5d	³ D ₃ - (² P)6p	³ D ₃	2	3340.057	29931.00	(² P)5d	³ F ₂ - (² P)6p	³ D ₁
5	3542.347	28221.81	(² D)6s	³ D ₃ - (² S)4f	³ F ₂	1	3339.497	29936.02	(² D)5d	³ P ₂ - (² D)4f	³ G ₃
4	3539.937	28241.02	(² S)4f	³ F ₃ - (² D)6d	³ P ₂	3	3338.987	29940.59	(² D)6s	³ D ₁ - (² P)6p	³ P ₁
4	3539.937	28241.02	(² P)5d	³ D ₂ - (² P)6p	³ S ₁	0	3336.237	29965.27	(² P)6p	³ P ₀ - (² D)7s	¹ D ₁
2	3531.817	28305.95	(² S)6d	³ D ₁ - 5s° 5p° 5s°	³ S ₀	3	3334.227	29983.34	(² P)6p	³ F ₂ - (² D)6d	¹ G ₃
0	3531.62	28307.55	(² P)5d	³ P ₁ - (² P)4f	³ D ₂	0	3331.646	30006.56	(² P)5d	³ D ₁ - (² S)4f	³ F ₃
4	3522.797	28378.42	(² S)5d	³ D ₁ - (² S)6p	³ P ₁	3	3326.387	30054.00	(² P)6p	³ F ₂ - (² D)6d	³ F ₃
3	3519.107	28408.18	(² D)6s	³ D ₂ - (² P)6p	³ P ₂	1	3320.067	30111.21	(² P)6s	³ P ₁ - (² D)4f	³ F ₃
4	3509.766	28483.78	(² P)5d	³ D ₂ - (² D)4f	³ D ₃	1	3320.067	30111.21	(² S)4f	³ F ₂ - (² D)6d	¹ F ₃
3	3501.647	28549.82	(² P)6p	³ D ₂ - (² D)7s	¹ D ₂	1	3319.547	30115.93	(² P)5d	³ D ₂ - (² P)6p	¹ D ₂
1	3494.817	28605.62	(² P)5d	³ F ₂ - (² S)4f	³ F ₂	2	3317.447	30134.99	(² S)5d	³ D ₁ - (² S)6p	³ P ₂
2	3494.506	28608.16	(² P)5d	³ D ₁ - (² P)6p	³ D ₂	2	3314.866	30158.45	(² D)5d	³ S ₁ - (² P)6p	³ D ₂
1	3488.127	28660.48	(² P)6p	³ D ₂ - (² D)6d	³ D ₃	1	3314.257	30163.99	(² S)4f	³ F ₃ - (² D)6d	¹ G ₃
1	3479.136	28734.54	(² D)6s	³ D ₁ - (² S)4f	³ F ₂	2	3306.797	30232.04	(² D)5d	³ S ₁ - (² P)6p	³ P ₁
1	3472.347	28790.72	(² P)6p	³ P ₁ - (² D)6d	³ D ₁	1	3306.457	30235.15	(² S)4f	³ F ₃ - (² D)6d	³ F ₃
4	3468.216	28825.01	(² S)6s	³ S ₂ - (² S)6p	³ P ₁	1	3304.047	30257.20	(² D)5d	³ S ₁ - (² P)6p	³ P ₀
4	3467.217	28933.32	(² D)5d	³ P ₁ - (² D)4f	¹ P ₁	2	3301.537	30280.20	(² S)6p	³ P ₂ - (² S)6d	³ D ₂

2	3295.937	30331.65	(² P)5d	¹ D ₂ - (² P)6p	³ D ₁	(² D)6s	³ D ₂ - (² P)6p	³ D ₁
1	3288.537	30399.90	(² S)4f	³ F ₃ - (² D)6d	³ D ₃	(² S)6p	³ P ₁ - (² S)6d	³ D ₂
2	3287.907	30405.73	(² P)6p	³ P ₁ - (² D)6d	³ P ₂	(² P)6p	³ F ₃ - (² D)6d	³ G ₅
1	3287.796	30406.75	(² S)6p	³ P ₂ - (² S)6d	³ D ₁	(² P)6p	³ F ₃ - (² D)6d	³ F ₂
1	3285.817	30425.07	(² S)6p	³ P ₁ - (² S)7s	³ S ₂	(² S)6p	³ P ₁ - (² S)7s	³ S ₂
1	3284.637	30436.00	(² P)6s	³ P ₁ - (² D)4f	³ S ₂	(² P)6s	³ D ₂ - (² P)6p	³ D ₁
2	3280.496	30474.41	(² D)5d	³ F ₃ - (² D)4f	³ G ₅	(² D)5d	³ D ₂ - (² S)4f	³ F ₂
0	3279.127	30487.14	(² P)5d	³ D ₁ - (² P)6p	³ P ₁	(² P)5d	³ P ₁ - (² S)6d	³ S ₁
2	3278.437	30493.55	(² S)6p	³ P ₂ - (² S)6d	³ D ₁	(² S)6p	³ F ₃ - (² D)6d	³ S ₁
2	3276.387	30512.63	(² P)5d	³ D ₂ - (² S)4f	³ F ₂	(² P)5d	³ P ₁ - (² S)6d	³ S ₁
0	3269.397	30577.87	(² D)5d	³ D ₃ - (² S)4f	³ F ₂	(² D)5d	³ D ₂ - (² P)6p	³ D ₁
4	3268.977	30581.79	(² S)6s	³ S ₂ - (² S)6p	³ S ₁	(² S)6s	³ G ₅ - (² P)6p	³ F ₂
2	3267.047	30599.86	(² P)5d	³ D ₁ - (² D)4f	³ P ₂	(² P)5d	³ P ₁ - (² D)4f	³ D ₂
0	3261.467	30632.21	(² P)6s	³ P ₁ - (² P)6p	³ S ₁	(² P)6s	³ F ₃ - (² D)6d	³ D ₁
2	3257.847	30686.27	(² D)6s	³ D ₂ - (² S)4f	³ F ₂	(² D)6s	³ P ₁ - (² P)6p	³ F ₂
0	3256.517	30698.80	(² P)5d	³ D ₁ - (² P)6p	³ P ₂	(² P)5d	³ D ₂ - (² D)7s	³ D ₂
2	3256.247	30701.35	(² P)5d	³ D ₂ - (² P)6p	³ D ₁	(² P)5d	³ P ₁ - (² P)6p	³ D ₂
2	3248.617	30773.45	(² P)6s	³ P ₂ - (² D)4f	³ P ₁	(² P)6s	³ F ₃ - (² P)6p	³ D ₂
3	3246.847	30790.23	(² D)5d	³ D ₃ - (² S)4f	³ F ₂	(² D)5d	³ F ₂ - (² P)6p	³ P ₁
2	3244.127	30816.04	(² P)6p	³ D ₁ - (² D)6d	³ P ₁	(² P)6p	³ P ₀ - (² P)6d	³ D ₁
5	3242.857	30828.11	(² S)5d	³ D ₃ - (² S)6p	³ P ₂	(² S)5d	³ P ₁ - (² P)6d	³ D ₁
2	3240.467	30850.85	(² P)6s	³ P ₂ - (² D)4f	³ F ₁	(² P)6s	³ D ₂ - (² P)6d	³ D ₁
3	3236.836	30885.45	(² S)5d	³ D ₁ - (² S)6p	³ P ₀	(² S)5d	³ P ₁ - (² S)6p	³ P ₂
2	3235.727	30896.04	(² P)6s	³ P ₂ - (² D)4f	³ D ₂	(² P)6s	³ D ₂ - (² S)6p	³ P ₁
2	3233.277	30919.45	(² P)5d	³ D ₁ - (² P)6p	³ P ₂	(² P)5d	³ P ₁ - (² S)6p	³ P ₁
2	3227.157	30978.08	(² S)6p	³ P ₀ - (² S)7s	³ S ₁	(² S)6p	³ P ₂ - (² D)4f	³ D ₂
1	3222.987	31018.16	(² P)6p	³ P ₁ - (² D)6d	³ S ₁	(² P)6p	³ F ₃ - (² D)4f	³ H ₅
1	3199.217	31248.62	(² D)5d	³ P ₁ - (² P)6p	³ P ₁	(² D)5d	³ F ₂ - (² D)7s	³ D ₃
3	3196.507	31275.11	(² D)5d	³ D ₁ - (² S)6p	³ P ₁	(² D)5d	³ P ₀ - (² D)6d	³ S ₁
3	3196.247	31277.65	(² D)5d	³ D ₂ - (² P)6p	³ P ₁	(² D)5d	³ D ₂ - (² P)6p	³ D ₁
3	3185.207	31386.06	(² P)6p	³ D ₂ - (² D)6d	³ D ₂	(² P)6p	³ P ₂ - (² D)4f	³ F ₂
2	3184.267	31395.32	(² P)6p	³ P ₁ - (² D)7s	³ D ₁	(² P)6p	³ F ₃ - (² D)4f	³ H ₅
1	3177.107	31466.07	(² P)6p	³ P ₁ - (² D)6d	³ F ₂	(² P)6p	³ P ₁ - (² S)6d	³ D ₂
1	3169.747	31539.13	(² D)6s	³ D ₃ - (² S)4f	³ F ₂	(² D)6s	³ F ₃ - (² D)6d	³ G ₅
2	3164.467	31591.75	(² P)6s	³ P ₀ - (² S)4f	³ F ₂	(² P)6s	³ D ₁ - (² P)6p	³ D ₂
1	3160.657	31629.84	(² P)6p	³ P ₁ - (² D)7s	³ D ₂	(² P)6p	³ D ₂ - (² D)7s	³ G ₅
1	3156.667	31669.81	(² D)5d	³ D ₂ - (² S)4f	³ F ₂	(² D)5d	³ S ₁ - (² P)6p	³ D ₁
2	3155.507	31681.46	(² D)5d	³ P ₁ - (² P)6p	³ P ₂	(² D)5d	³ F ₃ - (² D)6d	³ F ₂
2	3153.437	31702.25	(² P)6p	³ F ₃ - (² D)7s	³ D ₂	(² P)6p	³ D ₂ - (² D)4f	³ F ₂
2	3152.998	31706.67	(² D)6s	³ D ₂ - (² S)4f	³ F ₂	(² D)6s	³ P ₁ - (² S)6d	³ D ₃
2	3151.826	31718.45	(² P)5d	³ D ₁ - (² P)6p	³ P ₁	(² P)5d	³ D ₂ - (² S)6d	³ D ₃
3	3150.967	31727.10	(² D)5d	³ G ₅ - (² P)6p	³ F ₁	(² D)5d	³ P ₁ - (² P)6p	³ P ₁
3	3150.827	31728.51	(² S)6p	³ P ₂ - (² S)7s	³ S ₁	(² S)6p	³ P ₂ - (² S)7s	³ S ₂
2	3150.687	31729.92	(² P)5d	³ P ₂ - (² P)6p	³ S ₁	(² P)5d	³ P ₁ - (² D)6d	³ D ₂
2	3141.627	31821.42	(² S)5d	³ P ₂ - (² S)6p	³ P ₁	(² S)5d	³ D ₃ - (² D)4f	³ D ₂
4	3138.277	31855.39	(² P)6p	³ D ₂ - (² D)6d	³ F ₁	(² P)6p	³ F ₃ - (² D)7s	³ D ₃
0	3126.767	31972.65	(² P)5d	³ P ₂ - (² D)4f	³ D ₃	(² P)5d	³ P ₁ - (² S)7s	³ S ₁
1	3124.947	31991.27	(² P)6s	³ P ₁ - (² D)4f	³ P ₁	(² P)6s	³ P ₁ - (² D)6d	³ G ₅
0	3124.597	31994.85	(² P)5d	³ D ₂ - (² P)6p	³ P ₁	(² P)5d	³ F ₃ - (² D)7s	³ D ₃
2	3122.147	32019.96	(² P)5d	³ D ₃ - (² D)4f	³ P ₂	(² P)5d	³ F ₃ - (² D)4f	³ G ₅

1	2976.748	33583.91	(² P)6p	³ P ₂ - (² D)6d	³ D ₃	3	2912.377	34326.16	(³ S)6p	³ P ₂ - (³ S)6d	³ D ₃
1	2974.897	33604.80	(² P)5d	³ P ₂ - (² P)6p	¹ D ₂	3	2911.907	34331.70	(³ S)5d	³ D ₁ - (³ S)6p	³ P ₁
3	2971.527	33642.91	(² D)5d	³ G ₅ - (³ S)4f	³ F ₄	1	2911.477	34336.77	(² D)5d	³ S ₁ - (² P)6p	³ S ₁
1	2971.258	33645.96	(² D)5d	³ D ₁ - (³ S)4f	³ F ₂	2	2910.368	34349.86	(² P)6p	³ D ₂ - (² D)6d	³ F ₃
1	2971.167	33646.98	(² P)6p	³ D ₁ - (² D)7s	³ D ₁	0	2910.09	34353.17	(² P)5d	³ F ₃ - (³ S)5f	³ F ₄
4	2970.487	33654.69	(³ S)6p	³ P ₂ - (³ S)6d	³ D ₃	3	2906.557	34394.89	(² D)5d	³ G ₅ - (² P)6p	³ F ₄
1	2970.077	33659.33	(³ S)4f	³ F ₃ - (² D)7s	¹ D ₂	1	2904.168	34423.19	(² P)5d	³ D ₁ - (² D)4f	¹ D ₂
1	2970.077	33659.33	(³ S)4f	³ F ₃ - (² D)7s	³ D ₃	1	2902.287	34445.49	(² P)6p	³ P ₂ - (² D)6d	³ D ₂
4	2969.768	33662.84	(² D)5d	³ G ₅ - (³ S)4f	³ F ₄	0	2897.697	34500.05	(² P)5d	³ P ₁ - (² P)6p	³ D ₁
1	2969.427	33666.70	(² P)6p	³ F ₃ - (² D)6d	³ G ₅	2	2896.647	34512.56	(³ S)5d	³ D ₁ - (³ S)6p	³ P ₂
1	2968.567	33676.45	(³ S)4f	³ F ₃ - (² D)6d	³ D ₃	0	2896.067	34519.47	(² P)5d	³ D ₂ - (² D)4f	³ P ₂
1	2968.427	33678.04	(³ S)4f	³ F ₃ - (² D)7s	³ D ₃	1	2895.037	34531.75	(³ S)6p	³ P ₂ - (³ S)6d	³ D ₁
1	2966.917	33695.18	(³ S)4f	³ F ₃ - (² D)6d	³ G ₅	2	2891.717	34571.39	(² D)5d	³ F ₃ - (² P)6p	³ F ₂
1	2964.928	33717.79	(² P)6p	³ D ₂ - (² D)6d	³ F ₂	2	2889.967	34592.33	(² P)6p	³ P ₁ - (² D)6d	³ S ₁
2	2964.167	33726.44	(² P)6p	³ D ₃ - (² D)6d	³ F ₄	0	2886.93	34628.75	(² P)5d	³ F ₃ - (³ S)5f	³ F ₃
0	2960.867	33764.03	(² D)5d	³ P ₂ - (² P)6p	³ S ₁	2	2886.677	34631.75	(³ S)4f	³ F ₃ - (² D)6d	³ D ₂
2	2960.337	33770.07	(³ S)4f	³ F ₃ - (² D)6d	³ D ₃	1	2879.357	34719.79	(² P)6p	³ P ₁ - (² D)6d	³ P ₁
1	2960.067	33773.15	(² D)5d	³ P ₁ - (² D)4f	³ P ₂	0	2873.287	34793.13	(² P)5d	³ P ₀ - (² P)6p	³ D ₁
2	2959.357	33781.25	(³ S)6p	³ P ₀ - (³ S)6d	³ D ₁	0	2872.747	34799.67	(² D)5d	³ D ₃ - (² P)6p	³ D ₂
1	2959.277	33782.17	(² D)5d	³ P ₁ - (³ S)6p	³ P ₀	2	2871.687	34812.52	(² P)6p	³ D ₂ - (² D)6d	³ D ₂
4	2954.927	33831.90	(² D)5d	³ D ₁ - (² P)6p	³ P ₂	2	2871.687	34812.52	(² D)5d	³ G ₅ - (² P)6p	³ F ₃
1	2954.167	33840.60	(² P)6p	³ D ₃ - (² D)7s	¹ D ₂	2	2871.267	34817.61	(³ S)5d	³ D ₂ - (³ S)6p	³ P ₂
1	2954.097	33841.40	(² P)5d	³ F ₄ - (² D)4f	³ D ₃	2	2871.097	34819.67	(³ S)6p	³ P ₁ - (³ S)6d	³ D ₂
1	2953.938	33843.23	(² D)5d	³ G ₅ - (² P)6p	³ F ₄	0	2869.517	34838.84	(² P)6s	³ P ₁ - (² P)6p	³ P ₂
0	2953.857	33844.15	(² D)6s	³ D ₁ - (² P)6p	¹ D ₂	0	2868.447	34851.84	(² D)5d	³ D ₁ - (² P)6p	³ P ₁
0	2951.527	33870.87	(² P)6p	³ F ₄ - (² D)6d	³ F ₄	1	2864.617	34898.43	(² P)5d	³ D ₂ - (² D)4f	³ D ₁
3	2948.067	33910.62	(² D)5d	³ G ₅ - (² P)6p	³ D ₂	0	2863.857	34907.69	(² D)6s	³ D ₂ - (² P)6p	³ D ₂
3	2947.507	33917.06	(² P)6p	³ F ₄ - (² D)6d	¹ G ₅	3	2862.417	34925.25	(³ S)5d	³ D ₂ - (³ S)6p	³ P ₁
2	2945.227	33943.32	(² P)6p	³ P ₁ - (² D)6d	¹ G ₅	0	2856.67	34995.55	(² P)5d	³ F ₃ - (² P)4f	³ G ₃
1	2944.677	33949.66	(² P)6p	³ D ₃ - (² D)6d	³ P ₁	0	2850.267	35074.12	(³ S)6s	³ S ₁ - (² P)6p	³ F ₂
1	2944.557	33951.04	(² P)6p	³ D ₃ - (² D)6d	³ D ₃	3	2847.917	35103.06	(² D)5d	³ P ₂ - (² D)4f	¹ P ₁
1	2943.427	33964.07	(² D)5d	³ F ₃ - (² D)4f	³ D ₃	3	2847.667	35106.15	(³ S)5d	³ D ₂ - (³ S)6p	³ P ₂
1	2942.057	33979.89	(² P)6p	³ P ₁ - (² D)6d	³ P ₂	2	2845.057	35138.35	(³ S)4f	³ F ₃ - (² D)6d	³ D ₂
1	2941.387	33987.63	(² D)5d	³ G ₅ - (² P)6p	³ D ₃	0	2844.117	35149.96	(² D)5d	³ D ₂ - (² D)4f	³ G ₃
2	2940.207	34001.27	(² P)6p	³ D ₂ - (² D)6d	¹ G ₅	1	2838.807	35215.71	(² P)6p	³ F ₂ - (² D)7s	³ D ₁
1	2939.727	34006.82	(² D)5d	³ P ₂ - (² D)4f	³ D ₃	1	2833.117	35286.43	(² P)6p	³ F ₂ - (² D)6d	³ F ₂
1	2939.107	34013.99	(² P)6p	³ F ₃ - (² D)6d	³ F ₃	1	2832.967	35288.30	(² D)6s	³ D ₃ - (³ S)4f	³ F ₄
3	2937.567	34031.82	(² D)5d	³ G ₅ - (³ S)4f	³ F ₃	0	2832.827	35290.04	(² P)6p	³ P ₁ - (² D)6d	¹ D ₂
2	2935.857	34051.64	(³ S)4f	³ F ₃ - (² D)6d	³ F ₄	3	2827.457	35357.06	(³ S)5d	³ D ₃ - (³ S)6p	³ P ₂
1	2935.717	34053.27	(² P)6p	³ F ₃ - (² D)6d	³ P ₂	2	2825.988	35375.45	(³ S)6p	³ P ₂ - (³ S)6d	³ D ₂
2	2932.758	34087.63	(³ S)5d	³ D ₀ - (³ S)6p	³ P ₁	0	2825.417	35382.59	(² P)6s	³ P ₀ - (² P)6p	¹ P ₁
2	2932.087	34095.42	(² P)6p	³ F ₄ - (² D)6d	³ D ₃	2	2820.067	35449.71	(² P)6p	³ F ₂ - (² D)7s	³ D ₂
3	2930.267	34116.60	(³ S)4f	³ F ₄ - (² D)6d	³ G ₅	2	2817.357	35483.81	(² P)5d	³ P ₂ - (² P)6p	¹ P ₁
0	2927.127	34153.20	(² D)5d	³ P ₁ - (² D)4f	³ D ₁	2	2815.918	35501.95	(³ S)6p	³ P ₂ - (³ S)6d	³ D ₁
1	2926.067	34165.57	(³ S)4f	³ F ₃ - (² D)7s	¹ D ₂	0	2815.267	35510.15	(² P)6s	³ P ₁ - (² D)4f	³ D ₂
1	2923.957	34190.22	(² P)5d	³ P ₂ - (² P)6p	³ D ₃	2	2814.457	35520.37	(³ S)6p	³ P ₂ - (³ S)7s	³ S ₂
2	2923.527	34195.25	(² D)5d	³ G ₅ - (³ S)4f	³ F ₄	1	2811.607	35556.37	(³ S)6p	³ P ₁ - (³ S)6d	³ D ₂
2	2917.597	34264.75	(² D)5d	³ F ₄ - (² P)6p	³ F ₄	2	2810.457	35570.92	(² P)6p	³ F ₂ - (² D)6d	³ G ₃
1	2916.627	34276.14	(³ S)4f	³ F ₃ - (² D)6d	³ D ₃	0	2809.528	35582.69	(² D)6s	³ D ₂ - (³ S)4f	³ F ₃
1	2915.037	34294.84	(³ S)4f	³ F ₄ - (² D)6d	³ D ₃	2	2809.057	35588.65	(² D)6s	³ D ₁ - (³ S)4f	³ F ₃
2	2914.137	34305.43	(² D)5d	³ F ₂ - (² P)6p	³ D ₁	2	2809.057	35588.65	(³ S)6p	³ P ₂ - (³ S)6d	³ D ₁

1	2808.567	35594.86	(² P)6p	¹ F ₃ - (² D)7s	³ D ₃	0	2695.648	37085.83	(² D)6s	³ D ₁ - (² P)6p	³ D ₁
1	2808.457	35596.25	(² D)5d	¹ F ₃ - (² P)6p	¹ D ₂	0	2695.648	37085.83	(² S)4f	³ F ₂ - (² P)6d	³ D ₁
2	2807.218	35611.97	(² P)6p	¹ F ₃ - (² D)6d	¹ G ₃	0	2694.118	37106.89	(² P)6p	³ P ₁ - (² D)6d	³ P ₀
1	2806.397	35622.38	(² P)5d	¹ D ₂ - (² P)6p	¹ D ₂	2	2691.438	37143.84	(² P)6p	³ D ₁ - (² D)7s	³ D ₂
1	2805.088	35639.01	(² D)5d	³ P ₂ - (² P)6p	¹ D ₂	0	2691.217	37146.88	(² P)6p	³ D ₁ - (² D)6d	¹ F ₃
0	2802.187	35675.90	(² D)5d	³ S ₁ - (² D)4f	¹ P ₁	1	2685.507	37225.86	(² P)5d	³ P ₁ - (² P)6p	³ D ₂
2	2800.197	35701.25	(² S)6p	³ P ₁ - (² S)7s	³ S ₂	1	2678.547	37322.58	(² S)6p	³ P ₁ - (² S)6d	³ D ₁
1	2797.867	35730.98	(² D)5d	³ D ₁ - (² D)4f	¹ G ₃	1	2670.248	37438.58	(² D)6s	³ D ₁ - (² P)6p	¹ D ₂
2	2797.117	35740.56	(² S)6p	³ P ₁ - (² S)6d	¹ D ₀	1	2669.007	37455.98	(² S)5d	³ D ₁ - (² D)7s	³ D ₁
2	2794.837	35769.71	(² S)6p	³ P ₁ - (² S)6d	¹ D ₀	1	2669.007	37455.98	(² P)6p	³ F ₂ - (² D)6d	³ G ₃
0	2792.47	35800.07	(² D)5d	³ D ₁ - (² S)5f	¹ F ₁	0	2667.937	37471.00	(² S)4f	³ F ₃ - (² D)6d	¹ F ₃
1	2785.797	35885.78	(² P)5d	³ D ₂ - (² D)4f	¹ F ₃	2	2660.997	37568.72	(² D)5d	³ F ₂ - (² P)6p	³ D ₂
0	2785.328	35891.83	(² D)5d	³ D ₂ - (² P)6p	¹ D ₂	1	2659.358	37591.88	(² P)5d	³ P ₀ - (² P)6p	³ P ₁
2	2784.927	35896.99	(² P)6p	³ F ₂ - (² D)6d	³ P ₂	1	2658.267	37607.30	(² S)5d	³ D ₀ - (² S)6p	³ P ₁
2	2783.328	35917.62	(² P)6p	³ F ₂ - (² D)6d	³ P ₂	0	2641.128	37851.34	(² S)5d	³ D ₁ - (² S)6p	³ P ₁
1	2782.687	35925.89	(² S)4f	³ F ₂ - (² D)6d	¹ P ₁	0	2639.147	37879.74	(² P)6p	³ D ₁ - (² D)6d	³ D ₁
0	2782.297	35930.92	(² P)5d	³ D ₂ - (² D)4f	¹ D ₂	1	2634.207	37950.77	(² D)5d	³ P ₂ - (² P)6p	³ P ₂
1	2779.638	35965.30	(² D)5d	³ D ₂ - (² P)6p	³ P ₁	0	2626.978	38055.21	(² P)6p	³ F ₃ - (² D)6d	³ D ₃
1	2777.937	35987.31	(² P)6p	³ F ₂ - (² D)6d	³ F ₂	1	2624.517	38090.88	(² D)5d	³ S ₁ - (² P)6p	³ P ₁
1	2776.957	36000.01	(² D)5d	³ F ₂ - (² P)6p	³ F ₂	1	2619.848	38158.77	(² S)6p	³ P ₂ - (² S)6d	³ D ₂
0	2774.788	36028.16	(² P)6p	³ P ₁ - (² D)7s	¹ D ₂	1	2616.627	38205.73	(² D)5d	³ G ₃ - (² P)6p	³ F ₃
2	2772.397	36059.22	(² S)6p	³ P ₁ - (² S)6d	³ D ₂	0	2611.027	38287.67	(² P)6s	³ P ₀ - (² D)4f	³ D ₁
2	2772.397	36059.22	(² P)5d	³ F ₂ - (² P)6p	³ D ₂	0	2610.568	38294.41	(² P)6p	³ P ₁ - (² D)6d	³ P ₁
1	2769.167	36101.28	(² P)6p	³ F ₂ - (² P)6p	³ D ₂	0	2607.497	38339.50	(² S)6p	³ P ₁ - (² S)6d	³ D ₂
1	2766.177	36140.30	(² D)5d	³ F ₂ - (² P)6p	³ D ₂	1	2600.117	38448.31	5s 5p ³	³ P ₁ - (² S)6p	³ P ₁
0	2765.95	36143.30	(² D)5d	³ D ₂ - (² P)4f	³ G ₃	1	2595.027	38523.72	(² D)5d	³ S ₁ - (² P)6p	³ P ₂
0	2763.007	36181.76	(² D)5d	³ F ₂ - (² P)6p	³ D ₂	0	2594.528	38531.14	(² D)5d	³ G ₃ - (² S)4f	³ F ₂
1	2763.007	36181.76	(² D)5d	³ F ₂ - (² S)4f	³ F ₃	0	2591.688	38573.36	(² D)5d	³ G ₃ - (² S)4f	³ F ₃
2	2762.727	36185.43	(² P)6p	³ F ₂ - (² D)6d	³ D ₁	1	2591.238	38580.06	(² D)5d	³ F ₃ - (² D)4f	³ D ₂
2	2761.578	36200.49	(² D)5d	³ F ₂ - (² S)4f	³ F ₃	1	2590.418	38592.27	(² D)5d	³ G ₃ - (² S)4f	³ F ₃
1	2760.717	36211.77	(² P)6p	³ F ₂ - (² D)6d	³ D ₂	1	2578.618	38768.86	(² S)5d	³ G ₃ - (² P)6p	³ F ₃
1	2760.717	36211.77	(² D)5d	³ S ₁ - (² P)6p	¹ D ₂	0	2578.368	38772.62	(² D)5d	³ G ₃ - (² P)6p	³ F ₃
1	2759.187	36231.85	(² P)6p	³ D ₂ - (² D)6d	³ P ₂	1	2574.608	38829.24	(² P)6p	³ D ₂ - (² P)6d	³ D ₁
0	2757.558	36253.26	(² P)5d	³ F ₂ - (² D)4f	³ F ₂	1	2572.327	38863.66	(² P)6p	³ P ₁ - (² D)6d	¹ D ₂
1	2754.877	36288.53	(² S)6p	³ P ₁ - (² S)6d	³ D ₁	1	2572.327	38863.66	(² P)5d	³ D ₂ - (² P)6p	³ D ₁
2	2747.858	36381.23	(² D)5d	³ F ₂ - (² P)6p	³ F ₃	1	2570.257	38894.96	(² S)6s	³ S ₁ - (² P)6p	³ P ₁
2	2740.777	36475.21	(² D)5d	³ F ₂ - (² P)6p	³ F ₃	0	2568.807	38916.91	(² P)6p	³ F ₃ - (² D)6d	³ D ₂
0	2739.187	36496.38	(² S)4f	³ F ₂ - (² D)6d	¹ D ₂	0	2568.807	38916.91	(² D)5d	³ G ₃ - (² P)6p	³ D ₁
1	2736.988	36525.71	(² D)5d	³ F ₂ - (² P)6p	³ D ₂	0	2550.547	39195.51	(² D)5d	³ S ₁ - (² D)4f	³ D ₂
1	2728.197	36643.39	(² S)6s	³ S ₁ - (² P)6p	³ D ₂	0	2544.098	39294.87	(² P)5d	³ F ₂ - (² P)6p	³ D ₁
1	2727.197	36656.83	(² D)5d	³ G ₃ - (² P)6p	³ F ₃	0	2541.877	39329.19	(² D)6s	³ D ₂ - (² D)4f	³ D ₂
0	2725.687	36677.13	(² P)6p	³ D ₂ - (² D)6d	¹ D ₂	0	2541.028	39342.34	(² P)6p	³ F ₂ - (² D)7s	³ D ₃
1	2718.098	36779.54	(² P)6p	³ P ₂ - (² D)6d	¹ F ₃	0	2538.918	39375.03	(² P)5d	³ P ₂ - (² D)4f	¹ F ₃
0	2714.048	36834.42	(² P)5d	³ F ₂ - (² P)6p	³ S ₁	0	2536.868	39406.85	(² P)6p	³ F ₃ - (² D)6d	¹ F ₃
2	2713.388	36843.38	(² P)6p	³ D ₂ - (² D)6d	³ S ₁	2	2533.318	39462.07	(² S)5d	³ D ₁ - (² P)6p	³ F ₂
1	2710.94	36876.68	(² D)5d	³ P ₀ - (² S)5f	³ F ₁	1	2523.967	39608.25	(² S)5d	³ D ₁ - (² S)6p	³ P ₂
1	2708.447	36910.58	(² P)6p	³ D ₁ - (² D)7s	³ D ₁	1	2521.428	39648.14	(² D)6s	³ D ₃ - (² D)4f	³ G ₃
0	2704.408	36965.71	(² S)4f	³ F ₂ - (² D)6d	¹ F ₃	1	2515.117	39747.61	(² D)5d	³ F ₂ - (² P)6p	¹ F ₃
0	2701.497	37005.53	(² P)6p	³ P ₁ - (² S)7s	³ S ₁	0	2514.09	39763.89	(² P)5d	³ D ₃ - (² P)4f	³ F ₃
0	2696.507	37074.01	(² P)6p	³ F ₂ - (² D)6d	³ D ₂	0	2513.337	39775.76	(² P)6p	³ D ₂ - (² D)6d	³ P ₁
1	2696.507	37074.01	(² S)5d	³ D ₁ - (² P)6p	³ D ₁	0					

0	2511.288	39808.22	(² S)6p	³ P ₁ - (² S)6d	³ D ₁	1	2339.398	42732.94	(² P)6p	³ P ₁ - (² P)6d	³ D ₁
0	2509.74	39832.81	5s 5p ³	¹ P ₁ - (² P)4f	³ D ₁	10	2338.884	42742.34	(² P)5d	³ P ₁ - (² D)4f	¹ P ₁
1	2504.907	39909.61	(² D)6s	³ D ₁ - (² P)6p	³ P ₀	4	2333.555	42839.94	(² D)6s	¹ D ₂ - (² P)6p	¹ P ₁
1	2501.037	39971.36	(² D)5d	¹ P ₁ - (² P)6p	³ D ₁	0	2327.083	42972.26	(² D)5d	³ P ₁ - (² S)5f	¹ F ₁
12	2486.727	40201.37	(² S)5d	³ D ₂ - (² S)6p	³ P ₂	6	2323.455	43026.14	(² D)6s	³ D ₃ - (² D)4f	³ H ₀
11	2485.006	40229.20	(² D)6s	³ D ₃ - (² D)4f	³ G ₀	7	2320.992	43071.79	(² P)5d	³ F ₂ - (² D)4f	³ P ₂
11	2483.464	40254.18	(² D)5d	³ F ₃ - (² S)4f	³ F ₂	11	2316.583	43153.76	(² P)6p	³ F ₂ - (² D)6d	¹ F ₁
11	2479.876	40312.42	(² D)5d	³ D ₂ - (² D)4f	³ D ₃	13	2313.392	43213.29	5s 5p ³	³ P ₁ - (² S)6p	³ P ₁
9	2479.130	40324.56	(² S)6s	³ S ₁ - (² P)6p	³ P ₀	12	2312.276	43234.14	(² D)5d	¹ P ₁ - (² P)6p	³ D ₂
3	2477.062	40358.21	(² S)5d	³ D ₁ - (² S)6p	³ P ₀	1	2309.922	43278.20	(² P)5d	³ P ₁ - (² P)6p	¹ D ₂
9	2473.146	40422.12	(² D)5d	³ P ₂ - (² D)4f	³ D ₁	3	2306.212	43361.15	(² P)5d	³ D ₂ - (² P)4f	³ F ₂
11	2472.377	40434.68	(² D)5d	³ F ₃ - (² P)6p	³ F ₀	1	2305.502	43361.15	(² D)6s	³ D ₂ - (² P)6p	³ P ₁
12	2471.319	40452.00	(² S)5d	³ D ₃ - (² S)6p	³ P ₂	12	2303.735	43394.42	(² D)5d	³ F ₂ - (² P)6p	³ P ₁
11	2468.393	40499.94	(² D)5d	³ D ₁ - (² S)4f	³ F ₂	12	2303.735	43394.42	5s 5p ³	³ P ₁ - (² S)6p	³ P ₂
11	2463.557	40579.44	(² D)5d	³ F ₃ - (² P)6p	³ D ₃	13	2300.876	43448.33	(² D)6s	³ D ₁ - (² D)4f	³ F ₂
11	2463.061	40587.61	(² P)5d	³ F ₂ - (² P)6p	¹ P ₁	13	2300.716	43451.35	(² S)5d	³ D ₂ - (² P)6p	³ F ₂
12	2452.644	40759.98	(² D)5d	³ F ₃ - (² S)4f	³ F ₂	1	2298.540	43492.48	(² P)5d	³ F ₂ - (² D)4f	³ D ₁
11	2447.083	40852.60	(² D)5d	³ D ₃ - (² P)6p	¹ D ₂	13	2290.834	43638.77	(² D)6s	³ D ₂ - (² D)4f	³ G ₃
9	2446.503	40862.29	(² P)5d	³ P ₁ - (² D)4f	³ F ₂	5	2288.714	43692.65	(² P)5d	³ D ₂ - (² S)5f	³ F ₃
12	2441.523	40945.63	(² D)5d	³ F ₃ - (² P)6p	³ P ₂	11	2286.634	43718.91	(² D)6s	³ D ₃ - (² D)4f	³ D ₃
2	2439.516	40979.32	(² P)5d	³ F ₃ - (² P)6p	³ P ₂	12	2283.828	43772.63	(² D)5d	³ F ₀ - (² S)4f	³ F ₀
12	2436.491	41030.18	(² S)5d	³ D ₃ - (² P)6p	³ D ₂	0	2274.412	43967.41	(² P)5d	³ D ₂ - (² S)5f	³ F ₂
7	2423.918	41243.00	(² P)5d	³ F ₀ - (² D)4f	³ F ₂	1	2274.190	43971.70	(² P)6s	¹ P ₁ - (² P)4f	³ D ₂
12	2422.767	41262.59	(² S)6s	³ S ₁ - (² S)4f	³ F ₂	0	2272.609	43988.70	(² D)6s	³ D ₁ - (² P)6p	³ S ₁
10	2418.744	41331.22	(² D)5d	³ P ₂ - (² D)4f	³ P ₁	10	2271.055	44018.80	(² P)5d	³ D ₁ - (² P)6p	³ P ₀
12	2416.744	41365.41	(² S)5d	³ D ₃ - (² P)6p	³ F ₃	5	2269.625	44060.15	(² P)5d	³ D ₂ - (² P)4f	³ G ₃
5	2416.744	41365.41	(² D)5d	¹ F ₃ - (² D)4f	¹ F ₃	1	2258.847	44256.68	(² D)5d	³ D ₂ - (² P)6p	³ P ₂
11	2414.544	41403.10	(² P)5d	³ P ₁ - (² P)6p	³ S ₁	10	2249.630	44437.97	(² P)5d	³ F ₃ - (² D)4f	¹ F ₃
3	2414.230	41408.49	(² D)5d	³ P ₂ - (² D)4f	¹ F ₃	0	2247.335	44483.36	(² P)5d	³ F ₂ - (² D)4f	¹ F ₃
3	2414.230	41408.49	(² D)5d	³ D ₂ - (² D)4f	¹ P ₁	10	2245.280	44524.07	(² P)5d	³ F ₂ - (² D)4f	¹ D ₂
2	2414.104	41410.64	(² D)5d	¹ F ₃ - (² D)4f	¹ D ₂	0	2235.349	44721.86	(² D)5d	³ D ₁ - (² P)6p	³ D ₂
9	2412.505	41438.10	(² D)5d	³ D ₃ - (² P)6p	³ D ₃	10	2231.673	44795.52	(² D)5d	³ D ₁ - (² P)6p	³ P ₁
2	2406.229	41546.16	(² D)6s	¹ D ₂ - (² P)6p	³ D ₃	1	2230.419	44820.69	(² D)5d	³ D ₁ - (² P)6p	³ P ₀
11	2403.792	41588.28	(² P)5d	¹ D ₂ - (² P)6p	³ D ₂	3	2227.588	44877.64	(² P)6p	³ P ₀ - (² P)6d	³ D ₁
10	2397.566	41696.27	(² P)5d	³ P ₀ - (² P)6p	³ S ₁	3	2225.071	44928.41	(² P)6p	³ P ₀ - (² P)6d	³ D ₁
12	2394.083	41756.92	(² S)5d	³ D ₂ - (² P)6p	³ D ₁	17	2223.640	44957.33	(² D)5d	³ D ₂ - (² D)4f	³ D ₂
11	2392.376	41786.71	(² D)5d	³ G ₃ - (² S)4f	³ F ₀	6	2220.544	45019.99	(² S)5d	³ D ₁ - (² S)4f	³ F ₂
12	2389.301	41853.25	(² P)5d	³ D ₁ - (² P)4f	³ F ₂	2	2220.544	45019.99	(² S)5d	³ D ₂ - (² P)6p	³ D ₂
11	2385.902	41900.09	(² D)5d	³ G ₃ - (² S)4f	³ F ₂	13	2214.382	45145.26	(² S)5d	³ D ₃ - (² S)4f	³ F ₃
12	2385.673	41904.11	(² D)5d	³ S ₁ - (² D)4f	³ P ₁	0	2213.799	45157.14	(² P)5d	³ P ₁ - (² P)6p	¹ P ₁
12	2383.974	41946.77	(² P)5d	³ F ₃ - (² P)4f	³ G ₀	11	2210.420	45226.17	(² P)5d	³ D ₂ - (² D)4f	³ F ₂
10	2382.087	41967.19	5s 5p ³	³ P ₀ - (² S)6p	³ P ₁	5	2205.587	45325.27	(² S)5d	³ D ₃ - (² P)6p	³ F ₀
6	2379.783	42007.82	(² D)5d	³ F ₂ - (² P)6p	³ D ₃	5	2204.333	45351.04	(² D)6s	³ D ₃ - (² P)6p	¹ D ₂
1	2378.714	42026.69	(² D)5d	³ S ₁ - (² D)4f	¹ D ₂	0	2203.682	45364.44	(² D)6s	¹ D ₂ - (² D)4f	³ P ₂
12	2369.595	42188.42	(² D)5d	³ F ₂ - (² S)4f	³ F ₂	0	2202.695	45384.76	(² D)5d	³ G ₃ - (² S)4f	³ F ₂
12	2366.139	42262.94	(² P)5d	³ D ₂ - (² P)4f	³ F ₃	1	2199.514	45450.39	(² P)5d	³ P ₀ - (² P)6p	¹ P ₁
5	2359.159	42375.02	(² D)5d	³ D ₁ - (² P)6p	³ P ₂	10	2199.974	45455.09	(² P)6s	³ P ₂ - (² P)4f	³ D ₃
12	2355.176	42459.67	(² P)5d	³ D ₂ - (² S)5f	³ F ₂	10	2198.583	45469.64	(² S)5d	³ D ₃ - (² P)6p	³ D ₃
11	2353.336	42469.04	(² S)6s	³ S ₁ - (² P)6p	³ P ₁	12	2197.801	45485.82	(² D)5d	¹ P ₁ - (² P)6p	³ P ₁
12	2350.563	42529.98	(² D)5d	³ D ₂ - (² P)6p	³ D ₃	6	2194.292	45558.56	(² D)5d	³ F ₂ - (² S)4f	³ F ₃

9	2192.428	45597.28	(² D)5d	³ G ₃ - (² S)4f	³ F ₄	15	2029.216	49264.25	(² P)5d	³ P ₀ - (² D)4f	³ P ₁
12	2189.828	45651.42	(² S)5d	³ D ₃ - (² S)4f	³ F ₃	15	2026.062	49340.94	(² D)6s	³ D ₃ - (² P)6p	³ D ₂
3	2185.701	45751.90	(² P)5d	³ P ₂ - (² P)4f	³ F ₃	4	2021.422	49454.18	(² S)6p	³ P ₂ - (² D)6d	³ D ₂
2	2179.684	45863.84	(² D)6s	³ D ₁ - (² P)6p	³ D ₂	2	2021.956	49457.06	(² D)5d	³ S ₁ - (² P)4f	³ F ₂
16	2172.779	46009.58	(² P)5d	³ D ₂ - (² D)4f	³ D ₃	3	2021.566	49466.60	(² P)5d	³ D ₃ - (² P)4f	³ D ₂
7	2165.526	46163.67	(² D)5d	³ G ₃ - (² S)4f	³ F ₄	3	2018.714	49520.52	(² P)5d	³ D ₂ - (² P)6p	³ P ₁
7	2165.526	46163.67	(² S)5d	³ D ₁ - (² P)6p	³ P ₁	3	2018.562	49540.22	(² D)5d	³ F ₃ - (² P)4f	³ G ₃
10	2160.935	46261.74	(² P)5d	³ P ₁ - (² D)4f	³ D ₂	3	2016.825	49582.89	(² D)5d	³ P ₂ - (² P)4f	³ G ₃
15	2156.896	46348.36	(² D)5d	³ D ₂ - (² D)4f	³ P ₂	15	2013.859	49639.88	(² S)5d	³ D ₂ - (² S)4f	³ F ₂
13	2147.683	46547.15	(² S)5d	³ D ₁ - (² P)6p	³ D ₁	12	2006.317	49826.46	(² S)5d	³ D ₂ - (² P)6p	³ P ₂
0	2144.189	46623.00	(² D)5d	³ D ₃ - (² D)4f	³ F ₃	9	2001.085	49956.71	(² D)5d	³ G ₃ - (² D)4f	³ G ₃
2	2142.129	46667.82	(² D)5d	³ D ₃ - (² D)4f	³ D ₂	0	1997.497	50062.65	(² D)5d	³ S ₁ - (² S)5f	³ F ₂
13	2139.375	46727.90	(² D)5d	³ D ₂ - (² D)4f	³ D ₁	2	1997.330	50066.83	(² S)5d	³ D ₁ - (² P)6p	³ D ₂
13	2139.375	46727.90	(² D)5d	³ G ₃ - (² D)4f	³ G ₃	1	1989.377	50267.00	(² D)6s	³ D ₁ - (² D)4f	³ P ₂
13	2139.236	46730.93	(² D)6s	³ D ₂ - (² D)4f	³ F ₃	16	1985.405	50367.56	(² P)5d	³ D ₃ - (² P)4f	³ F ₂
2	2130.809	46915.73	(² D)5d	³ P ₁ - (² P)6p	³ P ₀	13	1983.985	50403.61	(² S)5d	³ D ₂ - (² P)6p	³ D ₂
1	2129.145	46967.20	(² P)5d	³ D ₃ - (² P)4f	³ D ₂	2	1980.606	50489.61	(² P)5d	³ D ₂ - (² P)4f	³ D ₃
1	2122.205	47105.90	(² P)5d	³ D ₂ - (² D)4f	³ P ₁	11	1979.266	50523.78	(² D)5d	³ G ₃ - (² D)4f	³ G ₃
15	2118.036	47198.62	(² S)5d	³ D ₂ - (² P)6p	³ F ₃	17	1978.705	50538.10	(² D)5d	³ G ₃ - (² D)4f	³ G ₃
15	2114.762	47271.68	(² S)5d	³ D ₂ - (² P)6p	³ P ₁	0	1974.445	50647.15	(² D)6s	³ D ₁ - (² D)4f	³ D ₁
1	2107.201	47456.31	(² P)5d	³ P ₂ - (² S)5f	³ F ₂	9	1973.829	50662.96	5s 5p ³	³ P ₀ - (² P)6p	³ D ₁
1	2099.545	47614.26	(² D)5d	³ F ₃ - (² S)4f	³ F ₂	7	1970.899	50738.26	(² S)5d	³ D ₂ - (² P)6p	³ F ₃
16	2096.570	47681.81	(² P)5d	³ P ₁ - (² D)4f	³ P ₂	9	1970.059	50759.90	(² S)5d	³ D ₃ - (² P)6p	³ D ₂
4	2095.350	47709.56	(² D)6s	³ D ₂ - (² D)4f	³ D ₃	0	1969.474	50774.98	(² D)5d	³ D ₁ - (² P)6p	³ D ₂
15	2095.126	47714.67	(² D)5d	³ D ₂ - (² D)4f	³ F ₃	8	1967.905	50815.46	(² P)5d	³ F ₃ - (² P)4f	³ F ₃
3	2094.527	47743.47	(² D)5d	³ F ₃ - (² P)4f	³ F ₃	0	1966.733	50845.75	(² S)5d	³ D ₂ - (² P)6p	³ P ₁
15	2092.661	47786.06	(² D)5d	³ F ₃ - (² P)4f	³ F ₃	14	1966.345	50855.78	(² P)5d	³ F ₂ - (² P)4f	³ F ₃
1	2085.124	47958.77	(² P)5d	³ P ₂ - (² S)4f	³ F ₃	15	1956.759	51104.92	(² D)5d	³ G ₃ - (² D)4f	³ G ₃
14	2083.751	47990.37	(² P)5d	³ D ₃ - (² P)4f	³ D ₃	3	1945.419	51402.81	(² D)5d	³ G ₃ - (² D)4f	³ G ₃
13	2079.995	48061.73	(² P)5d	³ P ₁ - (² D)4f	³ D ₁	12	1942.913	51469.11	(² P)6s	³ P ₁ - 5s ⁰ 5p ⁶ 1s ₀	³ S ₀
0	2077.610	48116.88	(² S)6s	³ S ₁ - (² S)4f	³ F ₂	13	1941.329	51511.11	(² D)5d	³ F ₃ - (² D)4f	³ H ₃
13	2075.090	48175.32	(² D)6s	³ D ₁ - (² P)6p	³ P ₂	7	1935.038	51678.58	(² D)6s	³ D ₁ - (² D)4f	³ D ₂
15	2072.866	48226.99	(² P)5d	³ D ₂ - (² P)6p	³ D ₃	16	1930.083	51811.25	(² S)5d	³ D ₁ - (² S)4f	³ F ₂
0	2072.247	48241.41	(² S)5d	³ D ₁ - (² P)6p	³ F ₂	11	1929.158	51836.09	(² D)5d	³ F ₃ - (² P)6p	³ D ₂
15	2067.384	48354.87	(² P)5d	³ P ₀ - (² D)4f	³ D ₁	1	1927.622	51877.40	(² P)6s	³ P ₁ - (² P)4f	³ D ₂
16	2061.175	48359.74	(² D)5d	³ D ₁ - (² D)4f	³ F ₂	2	1926.291	51913.24	(² P)5d	³ F ₃ - (² P)4f	³ F ₂
4	2061.362	48511.63	(² P)5d	³ D ₂ - (² P)4f	³ G ₃	15	1924.757	51954.60	(² D)5d	³ G ₃ - (² D)4f	³ G ₃
1	2060.385	48519.10	5s 5p ³	³ P ₂ - (² S)6p	³ P ₁	15	1924.757	51954.60	(² P)5d	³ F ₂ - (² P)4f	³ F ₂
14	2055.034	48645.42	(² D)5d	³ G ₃ - (² D)4f	³ H ₃	15	1924.197	51969.74	(² P)5d	³ F ₃ - (² S)5f	³ F ₂
16	2052.729	48700.03	5s 5p ³	³ P ₂ - (² S)6p	³ P ₂	15	1921.644	52038.77	5s 5p ³	³ P ₂ - (² S)6p	³ P ₁
13	2052.166	48713.39	(² D)5d	³ F ₃ - (² D)4f	³ G ₃	15	1916.211	52186.31	(² D)5d	³ F ₃ - (² D)4f	³ G ₃
5	2052.532	48720.31	(² D)5d	³ P ₁ - (² P)4f	³ D ₂	11	1915.595	52203.09	(² D)5d	³ F ₃ - (² D)4f	³ D ₃
14	2046.555	48846.93	(² D)6s	³ D ₁ - (² D)4f	³ D ₂	9	1912.564	52285.82	(² P)5d	³ F ₂ - (² S)5f	³ F ₃
1	2045.086	48897.70	(² D)5d	³ F ₃ - (² S)5f	³ F ₃	2	1911.131	52325.03	(² D)6s	³ D ₂ - (² D)4f	³ D ₂
2	2043.942	48925.07	(² P)5d	³ F ₃ - (² P)4f	³ F ₃	3	1910.626	52338.88	(² S)6s	³ S ₁ - (² P)6p	³ D ₂
9	2041.276	48973.24	(² D)5d	³ G ₃ - (² D)4f	³ H ₃	1	1907.038	52437.33	(² S)6s	³ S ₁ - (² P)6p	³ P ₀
16	2039.314	49020.36	(² S)5d	³ D ₃ - (² S)4f	³ F ₃	2	1904.599	52504.50	(² S)5d	³ D ₃ - (² S)4f	³ F ₂
15	2038.394	49042.48	(² D)5d	³ F ₂ - (² S)4f	³ F ₂	1	1901.779	52582.35	(² S)5d	³ D ₃ - (² P)6p	³ F ₃
12	2037.670	49059.89	(² D)5d	³ P ₁ - (² P)6p	³ P ₁	8	1900.693	52612.39	(² P)5d	³ F ₃ - (² P)4f	³ G ₃
15	2031.996	49196.86	(² D)5d	³ G ₃ - (² D)4f	³ H ₃	14	1899.216	52653.31	(² P)5d	³ F ₂ - (² P)4f	³ G ₃

14	1899.216	52653.31	(² D)5d	³ D ₁ - (² P)6p	¹ P ₁	9	1799.900	55558.64	(² D)5d	³ D ₁ - (² D)4f	³ D ₁
8	1899.156	52654.98	(² S)5d	³ D ₂ - (² P)6p	¹ P ₁	7	1799.769	55562.68	(² D)5d	³ S ₁ - (² P)4f	³ D ₂
18	1896.921	52717.02	(² S)5d	³ D ₃ - (² S)4f	³ F ₄	10	1799.691	55565.08	(² D)5d	³ F ₃ - (² D)4f	³ H ₆
16	1895.099	52767.68	(² D)5d	³ F ₃ - (² D)4f	³ G ₄	8	1789.258	55889.09	(² D)5d	³ D ₁ - (² P)4f	³ G ₃
2	1892.723	52833.94	(² S)5d	³ D ₃ - (² P)6p	¹ F ₃	4	1786.678	55969.79	(² D)5d	³ F ₃ - (² P)4f	³ D ₃
10	1888.374	52955.62	(² P)5d	³ P ₂ - (² P)4f	³ D ₂	3	1785.311	56012.64	(² D)5d	³ P ₂ - (² P)4f	³ D ₃
13	1888.083	52963.76	(² D)5d	³ P ₁ - (² P)6p	¹ D ₂	8	1784.661	56033.05	(² S)5d	³ D ₁ - (² P)6p	³ D ₃
18	1886.426	53010.29	(² S)5d	³ D ₃ - (² S)4f	³ F ₃	3	1780.067	56177.66	5s 5p ³	³ P ₀ - (² P)6p	³ P ₁
3	1882.957	53087.38	(² D)5d	³ D ₁ - (² P)6p	³ P ₂	10	1778.783	56218.22	(² D)5d	³ P ₁ - 5s ⁰ 5p ⁶	³ S ₀
2	1882.957	53107.97	(² D)6s	³ D ₂ - (² P)4f	³ F ₃	2	1778.425	56229.54	(² S)5d	³ D ₂ - (² P)6p	³ P ₁
9	1875.878	53308.36	(² S)5d	³ D ₁ - (² P)6p	³ D ₁	12	1777.910	56245.82	(² D)5d	³ G ₃ - (² P)6p	³ D ₃
13	1874.915	53335.76	(² D)5d	³ G ₃ - (² D)4f	³ H ₆	8	1777.551	56257.19	(² D)5d	³ F ₃ - (² D)4f	³ D ₃
11	1872.254	53411.57	(² P)5d	³ D ₂ - (² D)4f	³ F ₃	10	1775.174	56332.50	(² D)5d	³ G ₃ - (² D)4f	³ G ₃
10	1870.665	53456.94	(² P)5d	³ D ₂ - (² D)4f	³ D ₂	10	1774.033	56368.75	(² P)5d	³ F ₃ - (² P)4f	³ G ₃
0	1869.447	53491.76	(² S)5d	³ D ₁ - (² P)6p	³ P ₀	2	1770.919	56467.87	(² D)5d	³ D ₁ - (² D)4f	³ P ₁
15	1866.547	53574.85	(² D)5d	³ G ₃ - (² D)4f	³ H ₆	11	1770.174	56491.62	(² D)5d	³ F ₃ - (² P)4f	³ G ₃
14	1865.157	53614.80	(² D)5d	³ F ₃ - (² D)4f	³ G ₃	12	1770.099	56494.01	(² S)5d	³ D ₂ - (² S)4f	³ F ₂
7	1860.631	53745.21	(² D)6s	³ D ₂ - (² D)4f	³ P ₂	11	1767.089	56590.26	(² D)5d	³ D ₁ - (² D)4f	³ D ₂
10	1860.181	53758.21	(² D)5d	³ D ₁ - (² D)4f	³ D ₂	9	1760.178	56812.45	(² D)5d	³ G ₃ - (² P)6p	³ D ₃
11	1855.196	53902.66	(² D)5d	³ G ₃ - (² D)4f	³ H ₆	1	1759.622	56830.40	(² S)6s	³ S ₂ - (² D)4f	³ G ₃
15	1854.375	53926.53	(² D)5d	³ G ₃ - (² D)4f	³ H ₆	11	1757.396	56902.37	(² D)5d	³ F ₂ - (² D)4f	³ F ₂
14	1853.884	53940.82	(² P)5d	³ P ₂ - (² P)4f	³ G ₃	5	1752.318	57067.27	(² D)5d	³ G ₃ - (² D)4f	³ F ₃
11	1852.583	53978.68	(² P)5d	³ P ₂ - (² P)4f	³ D ₃	10	1752.022	57076.90	(² S)5d	³ D ₃ - (² D)4f	³ G ₃
9	1850.903	54027.68	(² D)5d	³ G ₃ - (² D)4f	³ D ₃	8	1750.609	57122.99	5s 5p ³	³ P ₁ - (² P)6p	³ F ₂
12	1848.989	54083.60	(² S)5d	³ D ₃ - (² S)4f	³ F ₃	10	1734.368	57657.90	(² S)5d	³ D ₃ - (² D)4f	³ G ₃
10	1848.695	54092.20	(² D)5d	³ D ₂ - (² P)4f	³ F ₃	4	1733.536	57685.55	(² D)5d	³ F ₂ - (² D)4f	³ D ₃
9	1837.300	54427.68	(² S)5d	³ D ₁ - (² P)6p	³ D ₃	8	1728.420	57856.31	(² S)6s	³ S ₁ - (² D)4f	³ P ₁
5	1837.223	54429.98	(² S)5d	³ D ₁ - (² S)4f	³ F ₃	7	1727.429	57889.49	(² D)5d	³ F ₃ - (² P)6p	³ D ₂
15	1835.811	54471.84	(² S)5d	³ D ₃ - (² S)4f	³ F ₃	6	1724.983	57971.60	(² D)5d	³ G ₃ - (² P)6p	³ P ₂
12	1835.532	54480.13	(² S)5d	³ D ₃ - (² S)4f	³ F ₃	2	1724.776	57978.54	(² S)5d	³ D ₃ - (² S)4f	³ F ₃
12	1834.255	54518.04	(² S)5d	³ D ₂ - (² S)4f	³ F ₃	4	1722.358	58059.92	(² P)5d	³ F ₂ - (² P)4f	³ D ₃
3	1833.588	54537.87	(² D)6s	³ D ₂ - (² S)5f	³ F ₃	14	1717.515	58223.66	(² P)5d	³ F ₃ - (² P)4f	³ F ₃
3	1831.680	54594.69	(² D)5d	³ G ₃ - (² D)4f	³ D ₃	6	1713.867	58347.59	(² D)5d	³ F ₃ - (² P)4f	³ F ₃
13	1830.939	54616.78	(² S)5d	³ D ₁ - (² P)6p	³ P ₂	10	1712.522	58393.42	(² S)5d	³ D ₂ - (² S)4f	³ F ₃
11	1827.883	54708.10	(² D)5d	³ P ₁ - (² S)4f	³ F ₃	10	1705.178	58644.89	(² S)5d	³ D ₃ - (² S)4f	³ F ₃
12	1827.367	54723.55	(² S)5d	³ D ₁ - (² S)4f	³ F ₃	2	1704.946	58652.88	(² D)6s	³ D ₃ - (² S)5f	³ F ₃
14	1826.490	54749.82	(² S)5d	³ D ₂ - (² P)6p	³ D ₂	2	1703.820	58691.66	5s 5p ³	³ P ₁ - (² P)6p	³ D ₂
14	1826.490	54749.82	(² S)5d	³ D ₃ - (² S)4f	³ F ₃	12	1699.515	58840.31	5s 5p ³	³ P ₀ - (² S)4f	³ F ₃
11	1825.867	54768.49	(² S)5d	³ D ₃ - (² S)4f	³ F ₃	3	1696.936	58929.74	(² D)5d	³ P ₁ - (² P)6p	³ D ₂
13	1823.391	54842.88	(² D)6s	³ D ₂ - (² P)6p	³ D ₃	3	1694.820	59003.30	(² D)5d	³ P ₁ - (² P)6p	³ P ₁
10	1821.334	54904.82	(² D)6s	³ D ₂ - (² P)4f	³ G ₃	3	1694.134	59027.21	(² D)5d	³ P ₁ - (² P)6p	³ P ₀
12	1819.857	54949.37	(² S)5d	³ D ₃ - (² P)6p	³ F ₃	6	1693.703	59042.24	(² D)5d	³ F ₃ - (² P)4f	³ D ₂
10	1817.397	55023.74	(² S)5d	³ D ₂ - (² S)4f	³ F ₂	3	1691.798	59108.71	(² D)6s	³ D ₁ - (² P)4f	³ F ₃
12	1815.085	55093.85	(² S)5d	³ D ₃ - (² P)6p	³ D ₃	6	1685.823	59318.20	(² D)5d	³ F ₂ - (² P)6p	³ D ₂
10	1814.503	55111.51	(² D)6s	³ D ₂ - (² D)4f	³ F ₃	2	1684.194	59375.59	(² P)6s	³ P ₁ - 5s ⁰ 5p ⁶	³ S ₀
3	1812.301	55178.48	(² D)5d	³ D ₁ - (² D)4f	³ P ₂	4	1678.873	59563.78	(² P)5d	³ F ₃ - (² P)4f	³ G ₃
12	1811.263	55210.08	(² S)5d	³ D ₂ - (² P)6p	³ P ₂	8	1675.824	59672.13	(² S)5d	³ D ₁ - (² D)4f	³ F ₂
10	1807.746	55317.51	(² S)5d	³ D ₂ - (² S)4f	³ F ₂	8	1674.633	59714.57	(² D)6s	³ D ₁ - (² S)5f	³ F ₂
6	1805.336	55391.36	(² S)5d	³ D ₀ - (² P)6p	³ P ₁	7	1673.566	59752.66	5s 5p ³	³ P ₀ - (² P)6p	³ P ₁
10	1804.117	55428.78	5s 5p ³	³ P ₁ - (² P)6p	³ D ₁	6	1672.557	59788.71	(² P)5d	³ D ₂ - (² P)4f	³ F ₃
11	1803.073	55460.87	(² S)5d	³ D ₃ - (² P)6p	³ P ₂	5	1669.355	59903.37	(² D)5d	³ F ₂ - (² P)6p	³ D ₃

0	1663.390	60118.18	(¹ S)6s	³ S ₁ - (² D)4f	³ F ₂	7	1557.460	64207.12	(¹ S)6s	³ S ₁ - (² D)4f	¹ D ₂
6	1661.093	60201.31	(² D)5d	³ F ₃ - (² P)6p	³ P ₂	9	1554.426	64332.43	5s 5p ³	³ P ₂ - (² P)6p	³ F ₃
2	1661.029	60203.63	(² D)5d	³ D ₃ - (² P)4f	³ D ₂	11	1553.907	64353.91	(¹ S)5d	³ D ₂ - (² D)4f	³ F ₂
5	1660.808	60211.67	(¹ S)5d	³ D ₁ - (² P)6p	³ S ₁	11	1551.651	64447.50	(² D)5d	³ P ₁ - (² D)4f	¹ P ₁
7	1656.612	60364.15	(¹ S)5d	³ D ₃ - (² D)4f	³ F ₂	10	1549.961	64517.77	5s 5p ³	³ P ₁ - (² P)6p	³ P ₁
1	1656.069	60383.96	(¹ S)5d	³ D ₃ - (² P)6p	¹ D ₂	10	1548.008	64599.14	(² D)5d	¹ G ₄ - (¹ S)5f	³ F ₄
8	1647.338	60704.01	(¹ S)6s	³ S ₁ - (² P)6p	³ P ₂	8	1547.346	64626.80	(² D)5d	³ D ₁ - (¹ S)5f	³ F ₄
7	1647.010	60716.09	(¹ S)5d	³ D ₂ - (² P)6p	³ D ₂	3	1540.970	64894.18	(¹ S)5d	³ D ₂ - (² P)6p	³ S ₁
6	1646.504	60734.75	5s 5p ³	³ P ₂ - (² P)6p	³ D ₁	6	1538.863	64983.05	(² D)5d	³ P ₁ - (² P)6p	¹ D ₂
8	1642.767	60872.91	(² D)5d	³ F ₃ - (² D)4f	³ D ₂	9	1538.220	65010.22	(² D)5d	³ F ₂ - (² D)4f	³ P ₁
2	1642.395	60886.68	(² P)5d	³ D ₂ - (² P)4f	³ F ₂	4	1536.812	65069.76	(¹ S)5d	³ D ₁ - (² D)4f	³ D ₂
2	1637.572	61066.01	(¹ S)5d	³ D ₂ - (² D)4f	¹ G ₃	9	1536.386	65087.81	(² D)5d	³ F ₂ - (² D)4f	¹ F ₃
8	1635.382	61147.81	(¹ S)5d	³ D ₃ - (² D)4f	³ D ₃	7	1535.328	65132.65	(² D)5d	³ F ₂ - (² D)4f	¹ D ₂
2	1634.072	61196.81	(² D)5d	³ F ₂ - (² P)6p	¹ P ₁	7	1535.224	65137.09	(¹ S)5d	³ D ₂ - (² D)4f	³ D ₃
5	1633.489	61218.65	(² P)5d	³ D ₂ - (¹ S)5f	³ F ₃	2	1533.416	65213.86	(² D)6s	³ D ₁ - (² P)4f	³ D ₂
7	1633.255	61227.42	(² D)5d	³ D ₁ - (² P)4f	³ D ₃	8	1532.765	65241.58	(² D)5d	¹ G ₄ - (² P)4f	¹ G ₃
7	1631.429	61295.96	(² D)5d	³ D ₂ - (² P)4f	³ D ₂	2	1530.558	65335.64	(¹ S)5d	³ D ₀ - (² P)6p	³ P ₁
5	1628.148	61419.48	(² P)5d	³ F ₃ - (² P)4f	³ F ₄	7	1526.586	65505.65	(¹ S)5d	³ D ₁ - (² P)6p	³ D ₂
7	1626.309	61488.93	(² D)6s	³ D ₂ - (² P)4f	³ F ₃	1	1524.280	65604.76	(¹ S)5d	³ D ₁ - (² P)6p	³ P ₀
4	1626.183	61493.68	(² P)5d	³ D ₂ - (¹ S)5f	³ F ₂	9	1521.501	65724.58	(² D)6s	³ D ₃ - (² P)4f	³ D ₃
6	1624.678	61550.66	(¹ S)5d	³ D ₁ - (² D)4f	¹ P ₁	8	1520.619	65762.71	(¹ S)5d	³ D ₃ - (² P)4f	³ D ₂
7	1623.748	61585.90	(² P)5d	³ D ₂ - (² P)4f	¹ G ₃	2	1515.558	65982.31	(² D)5d	³ F ₄ - (² P)4f	³ F ₃
7	1622.595	61629.67	(² D)5d	³ F ₂ - (² P)6p	³ P ₂	9	1511.119	66176.14	5s 5p ³	³ P ₂ - (² P)6p	¹ F ₃
7	1621.407	61674.84	(¹ S)5d	³ D ₀ - (¹ S)4f	³ F ₄	8	1509.841	66232.15	(¹ S)5d	³ D ₂ - (² D)4f	¹ P ₁
8	1619.484	61748.05	(² D)5d	³ D ₃ - (² P)4f	¹ G ₄	6	1509.530	66245.78	(² D)6s	³ D ₃ - (² P)4f	¹ G ₄
7	1616.083	61878.00	(¹ S)5d	³ D ₂ - (¹ S)4f	³ F ₂	10	1509.458	66248.96	5s 5p ³	³ P ₂ - (² P)6p	³ P ₁
6	1612.970	61997.45	(¹ S)6s	³ S ₂ - (² D)4f	¹ P ₁	9	1504.900	66449.59	(¹ S)5d	³ D ₂ - (² D)4f	³ G ₃
6	1612.970	61997.45	(² D)5d	³ G ₄ - (² D)4f	¹ F ₃	4	1503.997	66489.51	(¹ S)5d	³ D ₁ - (² D)4f	³ P ₂
4	1610.658	62086.42	(¹ S)5d	³ D ₁ - (² P)6p	¹ D ₂	5	1501.157	66615.30	(¹ S)5d	³ D ₁ - (² D)4f	³ G ₄
7	1605.322	62292.78	(² D)5d	³ F ₃ - (² D)4f	³ P ₂	1	1497.708	66768.67	(¹ S)5d	³ D ₂ - (² P)6p	¹ D ₂
8	1605.106	62301.19	(² D)5d	³ F ₂ - (² D)4f	³ D ₂	10	1495.446	66869.67	(¹ S)5d	³ D ₁ - (² D)4f	³ D ₁
6	1604.074	62341.26	(¹ S)5d	³ D ₂ - (¹ S)4f	³ F ₄	6	1488.474	67182.92	(¹ S)5d	³ D ₃ - (² D)4f	³ G ₄
8	1603.241	62373.67	5s 5p ³	³ P ₁ - (² P)6p	³ P ₀	9	1486.291	67281.56	(¹ S)5d	³ D ₃ - (² D)4f	³ G ₄
7	1601.817	62429.09	5s 5p ³	³ P ₂ - (² P)6p	³ F ₂	6	1484.688	67354.20	(¹ S)5d	³ D ₃ - (² P)6p	³ D ₃
8	1598.260	62568.05	(² D)5d	³ P ₁ - (² D)4f	³ F ₂	9	1482.243	67465.34	5s 5p ³	¹ S ₀ - 5s 5p ³	³ P ₁
8	1596.687	62629.68	(² P)5d	³ P ₁ - (² P)4f	³ D ₂	2	1474.781	67806.69	(² D)5d	³ G ₃ - (² P)4f	³ F ₃
8	1592.466	62795.69	(¹ S)6s	³ S ₁ - (² D)4f	³ P ₂	7	1472.727	67901.25	(¹ S)5d	³ D ₁ - (² D)4f	¹ D ₂
3	1589.351	62918.75	(² D)6s	³ D ₁ - (¹ S)5f	³ F ₃	9	1471.312	67966.57	(² D)5d	³ P ₁ - (² D)4f	³ D ₂
11	1585.770	63060.83	(² D)5d	³ S ₁ - 5s ⁰ 5p ⁶	¹ S ₀	6	1468.378	68102.35	(² D)6s	³ D ₃ - (² P)4f	³ F ₄
8	1584.577	63108.33	(² D)5d	³ P ₁ - (² P)6p	³ S ₁	9	1468.178	68111.62	5s 5p ³	³ P ₂ - (¹ S)4f	³ F ₃
9	1579.476	63312.15	5s 5p ³	³ P ₁ - (¹ S)4f	³ F ₂	4	1462.549	68373.79	(² D)5d	³ G ₄ - (² P)4f	³ F ₃
10	1578.154	63365.16	(¹ S)5d	³ D ₃ - (² P)6p	³ D ₃	8	1461.206	68436.61	5s 5p ³	³ P ₂ - (² P)6p	³ D ₃
9	1574.847	63498.22	5s 5p ³	³ P ₁ - (² P)6p	³ P ₂	7	1458.806	68549.23	(¹ S)5d	³ D ₃ - (² D)4f	¹ F ₃
9	1572.188	63605.62	5s 5p ³	³ P ₁ - (¹ S)4f	³ F ₁	9	1457.845	68594.40	(¹ S)5d	³ D ₃ - (² D)4f	¹ D ₂
8	1570.865	63659.19	(² D)5d	³ F ₃ - (² D)4f	¹ D ₂	7	1457.351	68617.66	5s 5p ³	³ P ₂ - (¹ S)4f	³ F ₂
8	1569.753	63704.28	(² D)5d	³ F ₂ - (² D)4f	³ P ₂	1	1455.769	68692.20	(² D)6s	³ D ₁ - (² P)4f	³ D ₂
9	1569.338	63721.14	(² D)5d	³ F ₂ - (² D)4f	³ P ₂	9	1453.408	68803.79	5s 5p ³	³ P ₂ - (² P)6p	³ P ₂
12	1562.547	63998.06	5s 5p ³	³ P ₂ - (² P)6p	³ D ₂	6	1451.141	68911.30	5s 5p ³	³ P ₂ - (¹ S)4f	³ F ₁
9	1562.006	64020.25	(² D)5d	³ D ₁ - (² P)4f	³ F ₂	6	1450.093	68961.10	(² D)5d	³ G ₃ - (¹ S)5f	³ F ₄
10	1560.437	64084.60	(¹ S)6s	³ S ₁ - (² D)4f	³ P ₁	6	1447.580	69080.82	(¹ S)5d	³ D ₂ - (² P)6p	³ P ₂
11	1560.011	64102.10	(² D)5d	³ F ₂ - (² D)4f	³ D ₁	3	1447.487	69085.26	(¹ S)5d	³ D ₂ - (² D)4f	³ H ₃

8	1446.268	69143.49	(³ S)5d	³ D ₁ - (² D)4f	³ F ₂	7	1316.442	75962.30	(³ S)5d	³ D ₁ - (² D)4f	³ P ₂
6	1441.199	69386.67	(³ D)5d	¹ P ₁ - (² D)4f	³ P ₂	0	1314.390	76080.92	(³ S)5d	³ D ₂ - (² S)5f	³ F ₆
5	1440.650	69413.11	(³ S)5d	³ D ₂ - (² D)4f	³ H ₆	8	1314.088	76098.41	(³ S)5d	³ D ₀ - (² D)4f	³ D ₁
8	1440.089	69440.17	(³ S)5d	³ D ₀ - (² P)6p	³ S ₁	7	1309.881	76342.84	(³ S)5d	³ D ₁ - (² D)4f	³ D ₁
6	1438.259	69528.49	(³ D)5d	³ G ₂ - (² S)5f	³ F ₆	10	1309.818	76346.46	5s ² 5p ¹ S ₀ - (² S)5d	³ D ₁	
7	1436.707	69603.61	(³ D)5d	³ G ₂ - (² P)4f	³ G ₂	1	1309.656	76355.92	(³ S)5d	³ D ₂ - (² S)5f	³ F ₃
6	1435.045	69684.23	(³ S)5d	³ D ₁ - (² P)6p	³ S ₁	8	1306.260	76554.46	(³ D)5d	³ G ₂ - (² P)4f	¹ G ₆
3	1434.820	69695.13	5s 5p ³	³ P ₀ - (² P)6p	³ S ₁	7	1305.721	76586.02	(³ D)5d	³ F ₆ - (² P)4f	³ F ₆
3	1433.956	69737.16	(³ S)5d	³ D ₂ - (² D)4f	³ F ₂	0	1305.475	76600.49	(³ D)5d	³ G ₂ - (² P)4f	³ D ₁
9	1432.185	69823.37	5s 5p ³	³ P ₂ - (² P)6p	³ P ₁	2	1303.385	76723.29	(³ S)5d	³ D ₂ - (² P)4f	³ G ₂
8	1428.810	69988.31	(³ S)5d	³ D ₂ - (² D)4f	³ F ₂	0	1299.234	76968.45	5s 5p ³	³ P ₂ - (² P)6p	³ D ₁
8	1427.844	70035.68	(³ D)5d	³ F ₂ - (² P)4f	³ F ₃	4	1294.672	77239.62	(³ D)5d	³ F ₃ - (² P)4f	³ D ₂
10	1425.999	70126.29	(² P)5d	³ P ₁ - 5s ⁰ 5p ⁶ S ₀	¹ S ₀	5	1294.477	77251.26	(³ S)5d	³ D ₁ - (² D)4f	³ P ₁
6	1425.200	70165.59	5s 5p ³	³ P ₁ - (² S)4f	³ F ₂	4	1292.427	77373.82	(³ S)5d	³ D ₁ - (² D)4f	¹ D ₂
8	1418.027	70520.51	(³ S)5d	³ D ₂ - (² D)4f	³ D ₂	9	1281.633	78025.43	5s 5p ³	³ P ₁ - (² D)4f	³ F ₂
8	1414.921	70675.30	(³ D)5d	¹ P ₁ - (² D)4f	³ P ₁	0	1278.311	78228.25	(³ D)5d	³ P ₁ - (² P)4f	³ F ₂
1	1413.006	70771.09	(³ S)5d	³ D ₂ - (² D)4f	³ D ₂	5	1277.742	78263.07	(³ D)5d	³ F ₃ - (² P)4f	³ D ₂
0	1412.846	70779.11	(³ S)5d	³ D ₀ - (² D)4f	¹ P ₁	8	1272.819	78565.77	5s 5p ³	³ P ₁ - (² P)6p	³ S ₁
9	1412.466	70798.14	(³ D)5d	¹ P ₁ - (² D)4f	¹ D ₂	3	1269.293	78784.02	(³ D)5d	³ F ₃ - (² P)4f	¹ G ₆
7	1407.990	71023.22	(³ S)5d	³ D ₁ - (² D)4f	³ P ₁	8	1267.171	78915.95	(³ S)5d	³ D ₂ - (² P)4f	³ F ₃
8	1405.042	71172.27	(³ S)5d	³ D ₂ - (² D)4f	³ P ₂	8	1253.650	79767.06	5s 5p ³	³ P ₂ - (² P)6p	³ P ₁
0	1404.681	71190.55	(³ D)5d	³ F ₃ - (² S)5f	³ F ₆	9	1251.484	79905.14	5s 5p ³	³ P ₁ - (² D)4f	³ P ₁
6	1402.224	71315.26	(³ S)5d	³ D ₀ - (² P)6p	¹ D ₂	9	1249.319	80043.61	5s 5p ³	³ P ₂ - (² D)4f	³ G ₂
7	1399.271	71465.79	(³ D)5d	³ F ₂ - (² P)4f	³ F ₃	0	1244.235	80370.66	(³ S)5d	³ D ₂ - (² S)5f	³ F ₁
7	1399.271	71465.79	(³ D)5d	³ F ₃ - (² S)5f	³ F ₃	9	1242.875	80458.63	5s 5p ³	³ P ₀ - (² D)4f	³ D ₁
5	1397.573	71552.63	(³ S)5d	³ D ₂ - (² D)4f	³ D ₁	0	1238.955	80713.18	(³ S)5d	³ D ₂ - (² P)4f	³ G ₂
1	1392.122	71832.78	(³ D)5d	³ F ₂ - (² P)4f	³ G ₂	12	1232.070	81164.24	5s ² 5p ¹	³ D ₂ - 5s 5p ³	³ P ₂
8	1391.936	71842.37	(³ S)5d	³ D ₀ - (² D)4f	¹ G ₆	2	1228.991	81367.53	5s 5p ³	³ P ₀ - (² D)4f	³ P ₁
9	1389.129	71987.53	5s 5p ³	³ P ₂ - (² S)4f	³ F ₃	0	1227.943	81437.00	(³ S)5d	³ D ₁ - (² P)4f	³ D ₂
8	1380.055	72460.90	(³ S)5d	³ D ₂ - (² D)4f	³ P ₁	12	1205.929	82923.60	5s ² 5p ¹	³ S ₀ - (² D)5d	¹ P ₁
6	1378.128	72562.23	(³ D)5d	³ F ₂ - (² P)4f	³ F ₂	0	1201.593	83153.65	(³ S)5d	³ D ₂ - (² P)4f	³ D ₂
8	1377.722	72583.58	(³ S)5d	³ D ₂ - (² D)4f	¹ D ₂	6	1200.033	83331.02	5s 5p ³	³ P ₂ - (² D)4f	³ F ₂
11	1375.295	72711.67	(³ D)6s	³ D ₁ - 5s ⁰ 5p ⁶ S ₀	¹ S ₀	9	1198.683	83424.86	5s 5p ³	³ P ₁ - (² D)4f	³ D ₂
6	1374.809	72737.36	(³ S)5d	³ D ₂ - (² P)6p	³ D ₂	2	1195.107	83674.55	(³ S)5d	³ D ₂ - (² P)4f	¹ G ₆
1	1370.076	72988.64	(³ S)5d	³ D ₂ - (² P)6p	³ D ₂	9	1188.853	84114.69	5s 5p ³	³ P ₂ - (² D)4f	³ D ₂
8	1366.709	73168.47	(³ D)5d	³ F ₂ - (² S)5f	³ F ₂	2	1186.249	84299.35	(³ S)5d	³ D ₂ - (² P)4f	³ F ₃
3	1364.977	73261.32	(³ D)5d	³ F ₂ - (² P)4f	³ G ₂	1	1185.767	84333.60	(³ D)5d	³ P ₁ - (² P)4f	³ D ₂
8	1356.358	73726.86	5s 5p ³	³ P ₂ - (² P)6p	³ D ₂	1	1182.729	84550.21	(³ S)5d	³ D ₂ - (² P)4f	³ F ₃
8	1355.012	73800.10	5s 5p ³	³ P ₀ - (² P)6p	³ S ₁	5	1179.186	84804.29	(³ S)5d	³ D ₁ - (² P)4f	³ F ₃
5	1347.545	74209.01	(³ D)5d	³ F ₂ - (² P)4f	³ D ₂	7	1178.630	84844.30	5s 5p ³	³ P ₁ - (² D)4f	³ P ₂
7	1344.320	74387.03	5s 5p ³	³ P ₁ - (² P)6p	³ D ₂	2	1177.617	84917.28	(³ S)5d	³ D ₀ - (² S)5f	³ F ₁
7	1342.928	74464.17	(³ S)5d	³ D ₂ - (² P)6p	³ P ₂	4	1174.243	85161.27	(³ S)5d	³ D ₁ - (² S)5f	³ F ₁
8	1342.534	74486.02	5s 5p ³	³ D ₁ - (² P)6p	³ P ₀	9	1173.857	85189.24	(³ S)5d	³ D ₂ - (² P)4f	³ F ₃
7	1341.518	74542.43	(³ D)5d	³ F ₂ - (² P)4f	¹ G ₆	2	1173.370	85224.64	5s 5p ³	³ P ₁ - (² D)4f	³ D ₁
6	1338.153	74729.85	(³ D)5d	³ F ₂ - (² P)4f	³ G ₂	9	1173.146	85240.89	(³ S)6s	³ S ₁ - 5s ⁰ 5p ⁶ S ₀	
8	1333.145	75010.60	(³ D)5d	³ G ₂ - (² P)4f	³ D ₂	2	1170.988	85397.97	(³ S)5d	³ D ₂ - (² P)4f	³ F ₂
5	1330.927	75135.60	(³ S)5d	³ D ₂ - (² D)4f	³ D ₂	1	1170.812	85410.79	(³ S)5d	³ D ₁ - (² S)5f	³ F ₂
3	1327.475	75331.01	(³ S)5d	³ D ₁ - (² P)4f	³ F ₂	9	1166.789	85705.29	(³ S)5d	³ D ₂ - (² S)5f	³ F ₆
7	1325.014	75470.91	5s 5p ³	³ P ₂ - (² S)4f	³ F ₂	9	1166.467	85728.92	(³ S)5d	³ D ₂ - (² S)5f	³ F ₃
2	1320.689	75718.03	(³ S)5d	³ D ₀ - (² D)4f	³ P ₂	0.5	1166.228	85746.53	5s 5p ³	³ P ₂ - (² P)6p	¹ D ₂
4	1316.873	75937.45	(³ S)5d	³ D ₁ - (² S)5f	³ F ₂	2	1163.061	85980.05	(³ S)5d	³ D ₂ - (² S)5f	³ F ₃

2	1160.992	86133.25	5s ² 5p ¹ 'P ₁ - ('D)4f 'P ₁	
6	1158.329	86331.26	5s ² 5p ¹ 'P ₂ - ('P)6p 'D ₃	
13	1156.475	86469.69	5s ² 5p ¹ 'D ₂ - 5s 5p ¹ 'P ₁	
10	1135.613	88058.15	5s ² 5p ¹ 'P ₂ - ('P)6p 'P ₂	
13	1130.348	88468.32	5s ² 5p ¹ 'P ₁ - 5s 5p ¹ 'P ₂	
2	1127.018	88729.74	5s ² 5p ¹ 'P ₂ - ('D)4f 'D ₂	
11	1124.428	88934.09	('S)5d 'D ₁ - 5s ⁰ 5p ¹ 'S ₀	
0	1109.257	90150.46	5s ² 5p ¹ 'P ₂ - ('D)4f 'P ₂	
3	1092.168	91561.03	5s ² 5p ¹ 'P ₂ - ('D)4f 'D ₂	
15	1088.954	91831.25	('D)5d 'P ₁ - 5s ⁰ 5p ¹ 'S ₀	
1	1077.844	92777.81	('S)5d 'D ₁ - ('P)4f 'D ₃	
13	1066.393	93774.02	5s ² 5p ¹ 'P ₁ - 5s 5p ¹ 'P ₂	
1	1060.529	94292.61	5s ² 5p ¹ 'P ₁ - ('S)5f 'F ₂	
9	1058.136	94505.83	5s ² 5p ¹ 'D ₂ - ('S)5d 'D ₃	
11	1055.326	94757.44	5s ² 5p ¹ 'D ₂ - ('S)5d 'D ₂	
11	1048.755	95351.18	5s ² 5p ¹ 'D ₂ - ('S)5d 'D ₁	
13	1047.799	95438.18	5s ² 5p ¹ 'P ₀ - 5s 5p ¹ 'P ₂	
13	1017.682	98262.53	5s ² 5p ¹ 'P ₂ - 5s 5p ¹ 'P ₂	
11	1016.188	98406.97	('S)5d 'D ₁ - 5s ⁰ 5p ¹ 'S ₀	
12	1014.825	98539.15	5s ² 5p ¹ 'P ₁ - 5s 5p ¹ 'P ₀	
6	1002.087	99791.73	5s ² 5p ¹ 'P ₂ - ('P)4f 'D ₂	
13	981.097	101926.76	5s ² 5p ¹ 'D ₂ - ('D)5d 'P ₁	
1	979.979	102043.00	5s ² 5p ¹ 'S ₀ - ('D)6s 'D ₁	
13	974.133	102655.36	5s ² 5p ¹ 'P ₁ - ('S)5d 'D ₁	
13	971.818	102899.93	5s ² 5p ¹ 'P ₁ - ('S)5d 'D ₀	
1	965.548	103568.15	5s ² 5p ¹ 'P ₂ - 5s 5p ¹ 'P ₁	
1	960.329	104131.00	5s ² 5p ¹ 'D ₂ - ('S)5d 'D ₃	
11	958.591	104319.79	5s ² 5p ¹ 'P ₀ - ('S)5d 'D ₁	
11	953.983	104823.72	5s ² 5p ¹ 'D ₂ - ('S)5d 'D ₁	
2	930.702	107445.73	5s ² 5p ¹ 'P ₁ - ('S)5d 'D ₂	
1	917.258	109020.64	5s ² 5p ¹ 'D ₂ - ('D)5d 'F ₃	
10	915.487	109231.47	5s ² 5p ¹ 'P ₁ - ('D)5d 'P ₁	
12	901.745	110896.08	5s ² 5p ¹ 'P ₀ - ('D)5d 'P ₁	
7	898.870	111250.77	5s ² 5p ¹ 'D ₂ - ('D)5d 'G ₃	
13	896.014	111605.39	5s ² 5p ¹ 'P ₂ - ('S)5d 'D ₃	
6	895.401	111681.76	5s ² 5p ¹ 'P ₁ - ('S)6s 'S ₂	
13	894.003	111856.51	5s ² 5p ¹ 'P ₂ - ('S)5d 'D ₂	
11	891.835	112128.36	5s ² 5p ¹ 'P ₁ - ('S)5d 'D ₁	
13	889.284	112450.01	5s ² 5p ¹ 'P ₂ - ('S)5d 'D ₁	
11	878.789	113793.00	5s ² 5p ¹ 'P ₀ - ('S)5d 'D ₁	
2	870.342	114897.41	5s ² 5p ¹ 'P ₁ - ('D)5d 'F ₂	
1	863.385	115823.17	5s ² 5p ¹ 'P ₁ - ('S)6s 'S ₁	
6	861.064	116135.44	5s ² 5p ¹ 'D ₂ - ('D)5d 'D ₁	
13	852.947	117240.61	5s ² 5p ¹ 'P ₂ - ('S)5d 'D ₂	
2	851.152	117487.77	5s ² 5p ¹ 'P ₀ - ('S)6s 'S ₁	
3	850.563	117569.23	5s ² 5p ¹ 'D ₂ - ('D)6s 'D ₁	
12	840.151	119026.19	5s ² 5p ¹ 'P ₂ - ('D)5d 'P ₁	
0	838.441	119268.99	5s ² 5p ¹ 'D ₂ - ('P)5d 'D ₂	
1	838.244	119297.00	5s ² 5p ¹ 'S ₀ - ('P)5d 'D ₁	
3	826.132	121046.00	5s ² 5p ¹ 'D ₂ - ('D)6s 'D ₁	
13	824.878	121230.09	5s ² 5p ¹ 'P ₂ - ('S)5d 'D ₃	

5s ² 5p ¹ 'P ₂ - ('S)6s 'S ₂	823.202	121476.86
5s ² 5p ¹ 'D ₂ - ('D)6s 'D ₃	822.640	121559.82
5s ² 5p ¹ 'P ₂ - ('S)5d 'D ₁	820.170	121926.00
5s ² 5p ¹ 'S ₀ - ('P)6s 'P ₁	811.135	122384.00
5s ² 5p ¹ 'P ₁ - ('D)5d 'D ₁	810.110	123439.97
5s ² 5p ¹ 'D ₂ - ('P)5d 'P ₁	808.859	123631.00
5s ² 5p ¹ 'P ₂ - ('D)5d 'F ₂	801.978	124691.64
5s ² 5p ¹ 'P ₁ - ('D)6s 'D ₂	800.835	124869.59
5s ² 5p ¹ 'D ₂ - ('D)5d 'D ₂	800.230	124964.00
5s ² 5p ¹ 'P ₀ - ('D)5d 'D ₁	799.333	125104.23
5s ² 5p ¹ 'P ₂ - ('S)6s 'S ₁	796.067	125617.50
5s ² 5p ¹ 'D ₂ - ('D)6s 'D ₂	793.968	125949.61
5s ² 5p ¹ 'D ₂ - ('D)5d 'D ₃	793.282	126058.53
5s ² 5p ¹ 'P ₂ - ('D)5d 'F ₃	792.896	126120.02
5s ² 5p ¹ 'P ₁ - ('P)5d 'D ₂	790.056	126573.24
5s ² 5p ¹ 'S ₀ - 5s 5p ¹ 'P ₁	784.788	127423.00
5s ² 5p ¹ 'D ₂ - ('P)5d 'F ₂	780.027	128200.62
5s ² 5p ¹ 'D ₂ - ('D)5d 'G ₃	779.782	128241.00
5s ² 5p ¹ 'P ₂ - ('D)5d 'G ₃	779.124	128349.33
5s ² 5p ¹ 'P ₁ - ('D)6s 'D ₁	779.124	128349.33
5s ² 5p ¹ 'P ₀ - ('D)6s 'D ₁	769.140	130015.33
5s ² 5p ¹ 'P ₁ - ('P)5d 'P ₀	765.442	130643.51
5s ² 5p ¹ 'D ₂ - ('D)5d 'S ₁	765.123	130698.00
5s ² 5p ¹ 'P ₁ - ('P)5d 'P ₁	763.729	130936.51
5s ² 5p ¹ 'D ₂ - ('D)5d 'P ₂	761.789	131270.00
5s ² 5p ¹ 'D ₂ - ('D)5d 'F ₃	761.532	131314.18
5s ² 5p ¹ 'P ₁ - ('D)5d 'D ₂	756.031	132269.67
5s ² 5p ¹ 'P ₀ - ('P)5d 'P ₁	754.142	132601.00
5s ² 5p ¹ 'P ₁ - ('D)6s 'D ₂	750.451	133253.23
5s ² 5p ¹ 'D ₂ - ('P)5d 'D ₂	750.160	133304.98
5s ² 5p ¹ 'D ₂ - ('P)6s 'P ₁	744.142	134382.88
5s ² 5p ¹ 'P ₂ - ('D)6s 'D ₂	742.570	134667.51
5s ² 5p ¹ 'P ₁ - ('P)5d 'F ₂	737.977	135505.56
5s ² 5p ¹ 'P ₂ - ('P)5d 'D ₂	733.314	136367.31
5s ² 5p ¹ 'D ₂ - ('P)5d 'D ₂	731.023	136794.58
5s ² 5p ¹ 'D ₂ - ('D)5d 'P ₁	727.042	137543.64
5s ² 5p ¹ 'P ₁ - ('D)5d 'S ₁	724.622	138003.00
5s ² 5p ¹ 'P ₂ - ('D)6s 'D ₁	723.872	138146.00
5s ² 5p ¹ 'D ₂ - ('P)5d 'D ₁	723.055	138302.00
5s ² 5p ¹ 'P ₁ - ('D)5d 'P ₂	721.631	138575.00
5s ² 5p ¹ 'P ₂ - ('D)6s 'D ₂	721.199	138658.05
5s ² 5p ¹ 'S ₀ - ('P)5d 'P ₁	719.694	138947.85
5s ² 5p ¹ 'D ₂ - ('P)5d 'D ₃	717.911	139292.99
5s ² 5p ¹ 'P ₀ - ('D)5d 'S ₁	715.984	139668.00
5s ² 5p ¹ 'P ₁ - ('P)5d 'P ₂	711.192	140609.00
5s ² 5p ¹ 'P ₁ - ('P)6s 'P ₀	710.680	140710.27
5s ² 5p ¹ 'P ₂ - ('P)5d 'P ₁	710.575	140731.06
5s ² 5p ¹ 'P ₁ - ('P)6s 'P ₁	705.777	141687.81
5s ² 5p ¹ 'D ₂ - ('P)6s 'P ₂	705.095	141824.94
5s ² 5p ¹ 'P ₂ - ('D)5d 'D ₂	703.906	142064.46
5s ² 5p ¹ 'D ₂ - ('P)6s 'P ₁	702.795	142289.00

5	699.069	143047.47	$5s^2 5p^3 P_2 - (^3D)6s^1 D_2$	5	536.524	186385.00	$5s^2 5p^3 P_2 - (^3S)6d^1 D_1$
12	698.550	143153.70	$5s^2 5p^3 P_2 - (^3D)5d^1 D_1$	4	535.475	186750.00	$5s^2 5p^3 P_2 - (^3D)6d^1 F_3$
7	697.584	143351.95	$5s^2 5p^3 P_0 - (^3P)6s^1 P_1$	2	534.536	187078.00	$5s^2 5p^3 P_1 - (^3D)6d^1 D_1$
10	693.971	144098.26	$5s^2 5p^3 P_1 - (^3P)5d^1 D_2$	2	529.956	188695.00	$5s^2 5p^3 P_1 - (^3D)6d^1 P_2$
8	691.036	144710.28	$5s^2 5p^3 D_2 - (^3D)5d^1 D_2$	1	529.827	188741.00	$5s^2 5p^3 P_0 - (^3D)6d^1 D_1$
10	690.400	144843.67	$5s^2 5p^3 P_1 - (^3D)5d^1 P_1$	1	528.234	189310.00	$5s^2 5p^3 P_1 - (^3D)6d^1 S_1$
1	688.239	145298.34	$5s^2 5p^3 P_2 - (^3P)5d^1 F_2$	2	524.257	190746.00	$5s^2 5p^3 P_1 - (^3D)7s^1 D_2$
10	688.044	145339.63	$5s^2 5p^3 P_2 - (^3P)5d^1 F_3$	1	523.645	190969.00	$5s^2 5p^3 P_0 - (^3D)6d^1 S_1$
5	686.794	145604.00	$5s^2 5p^3 P_1 - (^3P)5d^1 D_1$	0	521.314	191823.00	$5s^2 5p^3 P_1 - (^3D)6d^1 P_0$
11	685.599	145957.94	$5s^2 5p^3 D_1 - (^3P)5d^1 F_3$	1	520.194	192236.00	$5s^2 5p^3 P_1 - (^3D)6d^1 P_1$
13	682.926	146428.67	$5s^2 5p^3 D_2 - 5s 5p^3 P_1$	2	516.577	193582.00	$5s^2 5p^3 P_1 - (^3D)6d^1 D_2$
12	682.563	146506.63	$5s^2 5p^3 P_0 - (^3D)5d^1 P_1$	1	510.251	195982.00	$5s^2 5p^3 P_2 - (^3D)6d^1 F_2$
6	679.022	147270.71	$5s^2 5p^3 P_0 - (^3P)5d^1 D_1$	1	509.518	196264.00	$5s^2 5p^3 P_2 - (^3D)6d^1 G_2$
9	676.601	147797.64	$5s^2 5p^3 P_2 - (^3D)5d^1 S_1$	2	508.626	196608.00	$5s^2 5p^3 P_2 - (^3D)6d^1 F_3$
9	673.991	148369.91	$5s^2 5p^3 P_2 - (^3D)5d^1 P_2$	2	507.960	196866.00	$5s^2 5p^3 P_2 - (^3D)6d^1 D_1$
7	673.798	148412.52	$5s^2 5p^3 P_2 - (^3D)5d^1 F_3$	1	503.801	198491.00	$5s^2 5p^3 P_2 - (^3D)6d^1 P_2$
1	670.542	149133.00	$5s^2 5p^3 P_1 - (^3P)6s^1 P_2$	0	499.923	200031.00	$5s^2 5p^3 P_2 - (^3D)7s^1 D_3$
1	668.476	149593.93	$5s^2 5p^3 P_1 - (^3P)6s^1 P_1$	2	498.378	200651.00	$5s^2 5p^3 P_2 - (^3D)6d^1 D_3$
8	664.878	150403.51	$5s^2 5p^3 P_2 - (^3P)5d^1 P_2$	2	497.458	201022.00	$5s^2 5p^3 P_1 - (^3P)6d^1 D_1$
2	662.516	150939.80	$5s^2 5p^3 P_1 - (^3D)5d^1 P_0$	2	496.261	201507.00	$5s^2 5p^3 P_2 - (^3D)6d^1 D_2$
1	661.125	151257.37	$5s^2 5p^3 P_0 - (^3P)6s^1 P_1$	0	493.092	202802.00	$5s^2 5p^3 P_2 - (^3D)6d^1 P_1$
1	660.133	151484.63	$5s^2 5p^3 P_2 - (^3P)6s^1 P_1$	2	490.578	203841.00	$5s^2 5p^3 P_2 - (^3D)6d^1 F_3$
0	657.831	152014.84	$5s^2 5p^3 P_1 - (^3D)5d^1 D_2$				
12	650.479	153732.86	$5s^2 5p^3 P_1 - 5s 5p^3 P_1$				
10	646.667	154639.17	$5s^2 5p^3 P_2 - (^3D)5d^1 P_1$				
8	639.419	156391.99	$5s^2 5p^3 P_2 - (^3P)5d^1 D_3$				
1	633.088	157956.00	$5s^2 5p^3 D_2 - (^3P)5d^1 P_1$				
7	629.216	158927.94	$5s^2 5p^3 P_2 - (^3P)6s^1 P_2$				
1	627.403	159387.14	$5s^2 5p^3 P_2 - (^3P)6s^1 P_1$				
0	611.512	163529.00	$5s^2 5p^3 P_2 - 5s 5p^3 P_1$				
1	590.706	169289.00	$5s^2 5p^3 D_2 - (^3S)6d^1 D_3$				
3	574.739	173992.00	$5s^2 5p^3 P_1 - (^3S)7s^1 S_1$				
5	570.366	175326.00	$5s^2 5p^3 P_1 - (^3S)6d^1 D_2$				
1	569.291	175657.00	$5s^2 5p^3 P_0 - (^3S)7s^1 S_1$				
3	565.620	176797.00	$5s^2 5p^3 P_1 - (^3S)6d^1 D_1$				
5	560.356	178458.00	$5s^2 5p^3 P_0 - (^3S)6d^1 D_1$				
0	559.256	178809.00	$5s^2 5p^3 D_2 - (^3D)7s^1 D_1$				
0	559.031	178881.00	$5s^2 5p^3 D_2 - (^3D)6d^1 F_2$				
1	549.448	182001.00	$5s^2 5p^3 D_2 - (^3D)6d^1 S_1$				
4	548.444	182334.00	$5s^2 5p^3 P_2 - (^3S)6d^1 D_2$				
1	548.020	182475.00	$5s^2 5p^3 P_2 - (^3S)7s^1 S_2$				
1	548.020	182475.00	$5s^2 5p^3 P_2 - (^3S)6d^1 D_3$				
0	547.789	182552.00	$5s^2 5p^3 P_2 - (^3S)6d^1 D_1$				
5	544.108	183787.00	$5s^2 5p^3 P_2 - (^3S)7s^1 S_1$				
4	540.190	185120.00	$5s^2 5p^3 P_2 - (^3S)6d^1 D_2$				
1	538.491	185704.00	$5s^2 5p^3 D_2 - (^3D)6d^1 P_1$				
0	537.288	186120.00	$5s^2 5p^3 P_1 - (^3D)7s^1 D_1$				
1	537.106	186183.00	$5s^2 5p^3 P_1 - (^3D)6d^1 F_2$				
3	536.844	186274.00	$5s^2 5p^3 D_2 - (^3D)6d^1 D_2$				

Designation	$E(\text{cm}^{-1})$
$5s^2 5p^4 \quad 3p_2$	0.00 (86)
$3p_1$	9 794.36 (98)
$3p_0$	8 130.08 (79)
$1D_2$	17 098.73 (86)
$1S_0$	36 102.94 (78)
$5s^2 3p^4 (S) 6p \quad 5p_3$	149 061.57 (84)
$5p_2$	146 962.42 (66)
$5p_1$	146 781.48 (73)
$3p_2$	152 057.72 (64)
$3p_1$	150 301.10 (57)
$3p_0$	152 808.17 (89)
$(^2D) 6p \quad 3F_4$	166 554.82 (82)
$3F_3$	162 594.81 (56)
$3F_2$	160 691.30 (54)
$3D_3$	166 699.11 (66)
$3D_2$	162 259.97 (47)
$3D_1$	158 996.98 (38)
$3p_2$	167 066.32 (55)
$3p_1$	168 086.00 (62)
$3p_0$	165 941.69 (84)
$1F_3$	164 438.64 (49)

$5s^2 5p^6$	$5F_2$	197 860.38 (68)
	$5F_1$	197 611.00 (90)
	$1S_0$	210 857.49 (56)
$3F_4$	185 406.74 (42)	
$3F_3$	186 614.26 (67)	
$3F_2$	181 593.70 (41)	
$3D_3$	182 377.01 (42)	
$3D_2$	186 992.43 (25)	
$3D_1$	188 792.52 (92)	
$3P_2$	188 412.56 (38)	
$3P_1$	189 701.46 (79)	
$3P_0$		
$1H_5$	186 022.92 (62)	
$1G_4$	192 425.21 (76)	
$1F_3$	189 778.94 (55)	
$1D_2$	189 824.07 (50)	
$1P_1$	183 472.95 (70)	
$(^2P)4f$	$3G_3$	197 953.29 (29)
	$3F_4$	206 760.00 (30)
	$3F_3$	196 156.21 (51)
	$3F_2$	197 254.25 (43)
$3D_3$	204 382.87 (43)	
$3D_2$	203 359.91 (51)	
$3D_1$		
$1G_4$	204 904.40 (34)	
$5s^2 3p(^4S)5f$	$5F_5$	197 460.67 (89)
	$5F_4$	197 310.57 (74)
	$5F_3$	197 585.82 (56)

All levels are given in LS notation. The numbers in parentheses indicate the purities (in %) of the states

28

$3D_3$	156 392.68 (33)
$3D_2$	153 893.20 (28)
$3D_1$	155 400.90 (45)
$1D_2$	136 367.48 (22)
$3P_2$	150 404.24 (54)
$3P_1$	140 730.93 (44)
$3P_0$	140 437.79 (42)
$1P_1$	175 050.83 (64)

Table IV. Comparison between observed and calculated energy-level values (in cm^{-1}) and calculated percentage compositions for the $5s^2 5p^4 + 5s^2 5p^3(6p+4f+5f) + 5s^0 5p^6 + (5s5p^4 5d)$ configurations of Xe III. Eigenvector components larger than 5% are given. Observed [3] and calculated g_J factors are listed

J	E(obs.)	E(calc.)	Obs.-Calc.	$g_J(\text{obs.})$	$g_J(\text{calc.})$	Percentage composition
6	186 087	185 871	215		1.167	100 (2D) $4f^3H$
5	166 744	166 592	152		1.37	84 (4S) $4f^5F$ + 11 (2P) $4f^3G$
	181 357	181 345	12		1.11	36 (2D) $4f^3H$ + 22 (2D) $4f^1H$ + 17 (2P) $4f^3G$ + 15 (2D) $4f^3G$ + 9 (4S) $4f^5F$
	184 115	184 477	-363		1.18	81 (2D) $4f^3G$ + 13 (2D) $4f^3H$
	186 023	186 324	-301		1.01	62 (2D) $4f^1H$ + 38 (2D) $4f^3H$
	197 461	197 583	-123		1.38	89 (4S) $5f^5F$ + 7 (2P) $4f^3G$
4	166 355	166 084	271		1.30	64 (4S) $4f^5F$ + 17 (2D) $6p^3F$ + 7 (2P) $4f^3F$ + 5 (2P) $4f^3G$
	166 555	166 999	-444		1.26	82 (2D) $6p^3F$ + 13 (4S) $4f^5F$
	173 947	174 182	-235		1.21	65 (4S) $4f^3F$ + 9 (2D) $4f^3F$ + 8 (4S) $4f^5F$ + 6 (2D) $4f^3H$ + 6 (2P) $4f^1G$
	178 887	179 265	-378		1.11	58 (2D) $4f^3G$ + 9 (4S) $4f^5F$ + 6 (2P) $4f^3G$ + 6 (2P) $4f^1G$ + 6 (4S) $4f^3F$ + 6 (2P) $4f^3F$ + 5 (2D) $4f^3F$
	181 685	181 834	-149		0.96	56 (2D) $4f^3H$ + 23 (2D) $4f^3F$ + 8 (2P) $4f^3G$
	185 407	185 544	-137		1.14	42 (2D) $4f^3F$ + 20 (2D) $4f^3H$ + 16 (2D) $4f^3G$
	192 425	192 122	303		1.03	76 (2D) $4f^1G$ + 6 (2D) $4f^3G$ + 5 (2D) $4f^3F$
	197 311	197 619	-309		1.31	74 (4S) $5f^5F$ + 8 (2P) $4f^3G$
	204 904	205 178	-273		1.06	34 (2P) $4f^1G$ + 17 (2P) $4f^3G$ + 9 (2P) $4f^3F$ + 7 (4S) $5f^3F$ + 7 (4S) $4f^3F$
	206 760	206 576	184		1.11	30 (2P) $4f^1G$ + 30 (2P) $4f^1G$ + 10 (2D) $4f^1G$ + 9 (2D) $4f^3G$ + 7 (2P) $4f^3G$ + 5 (2D) $4f^3F$
3	149 062	148 836	225	1.57	1.61	84 (4S) $6p^5P$ + 12 (2P) $6p^3D$
	162 595	162 680	-85		1.16	56 (2D) $6p^3F$ + 17 (2D) $6p^1F$ + 14 (2P) $6p^3D$ + 10 (4S) $6p^5P$
	164 439	164 862	-424		1.13	49 (2D) $6p^1F$ + 32 (2D) $6p^3D$ + 16 (2D) $6p^3F$
	166 374	166 433	-59		1.20	74 (4S) $4f^5F$ + 7 (2P) $4f^3F$
	166 699	166 812	-113		1.23	66 (2D) $6p^3D$ + 21 (2D) $6p^1F$ + 12 (2D) $6p^3F$
	170 250	170 166	85		1.05	42 (4S) $4f^3F$ + 12 (2D) $4f^3F$ + 11 (2P) $4f^1F$ + 10 (2D) $4f^3G$ + 8 (4S) $4f^5F$ + 5 (2P) $4f^3D$ + 5 (2P) $4f^3G$
	178 306	178 780	-474		0.89	51 (2D) $4f^3G$ + 13 (4S) $4f^3F$ + 12 (2P) $4f^3G$ + 6 (4S) $4f^5F$
	182 377	181 721	656		1.25	42 (2D) $4f^3D$ + 12 (2P) $4f^3D$ + 12 (4S) $4f^3F$
	184 594	184 505	90		1.27	57 (2P) $6p^3D$ + 9 (2D) $6p^3F$ + 8 (2D) $4f^3D$ + 7 (2D) $6p^1F$
	186 614	186 511	103		1.10	67 (2D) $4f^3F$ + 15 (4S) $4f^3F$ + 7 (2P) $4f^3F$ + 5 (2D) $4f^3D$
	189 779	189 591	188		1.03	55 (2D) $4f^1F$ + 18 (2P) $4f^1F$ + 9 (2D) $4f^3D$
	196 156	196 050	106		1.11	51 (2P) $4f^3F$ + 17 (2P) $4f^3D$ + 12 (2P) $4f^1F$ + 6 (4S) $5f^5F$
	197 586	197 456	129		0.96	56 (4S) $5f^5F$ + 21 (2P) $4f^3G$
	197 953	197 931	23		1.11	29 (2P) $4f^3G$ + 25 (4S) $5f^5F$ + 16 (2P) $4f^1F$ + 12 (2D) $4f^1F$ + 8 (2D) $4f^3G$
	204 383	204 551	-168		1.22	43 (2P) $4f^3D$ + 24 (2D) $4f^3D$ + 14 (2P) $4f^1F$ + 6 (2P) $3f^3F$

2	0	-146	146		1.44	$86 p^4 3p + 11 p^4 1D$	
	17 099	17 246	-148		1.06	$86 p^4 1D + 11 p^4 3p$	
	146 962	146 789	173	1.70	1.67	$66 (4S)6p^5P + 14 (4S)6p^3P + 7 (2P)6p^3P + 6 (2P)6p^3D$	
	152 058	151 885	173	1.50	1.48	$64 (4S)6p^3P + 19 (4S)6p^5P + 8 (2P)6p^1D$	
	160 691	160 864	-173		0.95	$54 (2D)6p^3F + 15 (2D)6p^3D + 10 (4S)6p^3P + 9 (2P)6p^3D$	
	162 260	162 342	-82		1.18	$47 (2D)6p^3D + 16 (2D)6p^3F + 10 (2P)6p^3P + 10 (2D)6p^3P + 6 (2P)6p^1D + 6 (4S)6p^5P$	
	166 880	166 832	48		1.02	$81 (4S)4f^5F + 7 (2P)4f^3D$	
	167 066	167 057	9		1.36	$55 (2D)6p^3P + 20 (2D)6p^3D + 10 (2D)6p^1D + 5 (2P)6p^3P$	
	171 990	172 231	-242		1.10	$70 (2D)6p^1D + 20 (2D)6p^3P$	
	173 734	173 626	108		0.72	$77 (4S)4f^3F + 6 (2P)4f^3F + 5 (2P)4f^1D$	
	177 956	177 530	426		1.18	$59 (2P)6p^3D + 19 (2P)6p^1D + 14 (2P)6p^3P$	
	181 594	181 005	588		0.86	$41 (2D)4f^3F + 15 (2D)4f^1D + 14 (2D)4f^3D + 7 (2P)4f^1D + 7 (2P)4f^3D + 6 (4S)4f^5F$	
	184 009	183 888	121		1.00	$44 (2P)6p^1D + 17 (2P)6p^3D + 14 (2D)6p^3F + 8 (2D)4f^3F$	
	186 321	186 108	213		1.34	$27 (2P)6p^3P + 27 (2D)4f^3P + 11 (2P)6p^1D + 7 (2D)6p^3D$	
	186 992	187 118	-125		1.03	$31 (2D)4f^3F + 25 (2D)4f^3D + 12 (2P)6p^3P + 10 (2D)4f^1D + 6 (2P)4f^3D$	
	188 413	188 681	-268		1.28	$38 (2D)4f^3P + 25 (2D)4f^3D + 12 (2P)6p^3P + 8 (2P)4f^3D$	
	189 824	190 397	-573		1.10	$50 (2D)4f^1D + 21 (2D)4f^3D + 7 (2D)4f^3P$	
	197 254	197 145	109		0.81	$43 (2P)4f^3F + 22 (4S)5f^5F + 17 (4S)5f^3F + 6 (2P)4f^3D$	
	197 860	197 695	165		0.94	$68 (4S)5f^5F + 11 (2P)4f^3F + 7 (4S)5f^3F$	
	203 360	202 682	678		1.10	$51 (2P)4f^3D + 16 (2D)4f^3P + 13 (4S)5f^3F + 7 (2D)4f^1D$	
1	9 794	9 739	55		1.50	$98 p^4 3p$	
	146 781	146 609	173	2.28	2.19	$73 (4S)6p^5P + 9 (4S)6p^3P + 6 (2P)6p^3P$	
	150 301	150 097	204	1.59	1.55	$57 (4S)6p^3P + 14 (4S)6p^5P + 10 (2P)6p^1P + 6 (2D)6p^3P$	
	158 997	159 349	-352		1.01	$38 (2D)6p^3D + 26 (2D)6p^1P + 12 (4S)6p^3P + 5 (4S)6p^5P$	
	164 512	164 853	-341		0.97	$41 (2D)6p^1P + 32 (2D)6p^3D + 8 (2P)6p^3S + 6 (2P)6p^3D + 6 (2D)6p^3P + 5 (4S)6p^3P$	
	167 174	166 984	190		0.06	$87 (4S)4f^5F + 10 (2P)4f^3D$	
	168 086	168 301	-215		1.42	$62 (2D)6p^3P + 12 (2D)6p^1P + 11 (4S)6p^3P + 5 (2P)6p^3S$	
	175 231	175 094	137		0.66	$66 (2P)6p^3D + 20 (2P)6p^1P + 6 (2D)6p^1P$	
	178 029	177 703	327		1.40	$59 (2P)6p^3P + 18 (2P)6p^1P + 12 (2P)6p^3S + 7 (2P)6p^3D$	
	182 134	181 990	144		1.80	$58 (2P)6p^3S + 17 (2D)6p^3P + 11 (2P)6p^3P + 7 (2D)6p^1P$	
	183 473	183 352	121		0.91	$70 (2D)4f^1P + 12 (2P)4f^3D$	
	185 888	186 233	-345		0.99	$37 (2P)6p^1P + 15 (2P)6p^3P + 14 (2D)6p^3D + 8 (2P)6p^3D$	
	188 793	188 447	345		0.54	$92 (2D)4f^3D$	
	189 701	190 482	-780		1.37	$79 (2D)4f^3P + 10 (2D)4f^1P + 5 (2P)4f^3D$	
	197 611	197 587	24		0.05	$90 (4S)5f^5F + 7 (2P)5f^3D$	
0	8 130	8 271	-141			$79 p^4 3p + 19 p^4 1S$	
	36 103	36 012	91			$78 p^4 1S + 19 p^4 3p$	
	152 808	152 577	231			$89 (4S)6p^3P + 6 (2P)6p^3P$	

165 942	166 239	-297	84 (2D) $6p^3P$ + 13 (2P) $6p^1S$
178 055	177 654	400	83 (2P) $6p^3P$ + 13 (2P) $6p^1S$
190 491	190 484	7	67 (2P) $6p^1S$ + 15 (2D) $6p^3P$ + 7 (4S) $6p^3P$ + 6 (2P) $6p^3P$ + 5 (2D) $4f^3P$
	191 529		91 (2D) $4f^3P$
210 857	210 861	-3	56 $p^6\ ^1S$ + 39 (1D) $5d^1S$

Mean error of the least-squares fit $\sigma = [\sum (E_{\text{obs}} - E_{\text{calc}})^2 / (N-P)]^{1/2} = 331 \text{ cm}^{-1}$ with $N=73$ known levels and $P=22$ adjustable parameters.

Table V. Energy parameters (in cm^{-1}) for the $5s^25p^4 + 5s^23p^3(6p+4f+5f) + 5s^05p^6 + 5s5p^5d$ configurations of Xe III

Parameter	HF(E_{av})	Fitted	Fitted/HF			
p^4						
E_{av}		16905±160				
$F^2(5p,5p)$	50596	43681±1300	0.863±0.026	$F^2(5p,5f)$	12582	12582 (fix)
ζ_{5p}	6626	7995±300	1.207±0.045	$G^2(5p,5f)$	8811	8811 (fix)
$6p$				$G^4(5p,5f)$	6274	6274 (fix)
E_{av}		167407±70		ζ_{5p}	7102	7102 (fix)
$F^2(5p,5p)$	52840	39889±630	0.755±0.012	ζ_{5f}	33	33 (fix)
$F^2(5p,6p)$	12549	11964±760	0.953±0.061	p^6		
$G^0(5p,6p)$	2072	2007±80	0.969±0.039	E_{av}		251540±590
$G^2(5p,6p)$	2982	2443±600	0.819±0.200	$5d$		
ζ_{5p}	7301	8688±150	1.190±0.021	E_{av}		263000 (fix)
ζ_{6p}	939	1526±120	1.625±0.130	$F^2(5p,5p)$	51463	41170 (fix)
$4f$				$F^2(5p,5d)$	36501	36501 (fix)
E_{av}		187817±110		$G^1(5s,5p)$	68320	68320 (fix)
$F^2(5p,5p)$	51553	38033±720	0.738±0.014	$G^1(5s,5d)$	26862	26862 (fix)
$F^2(5p,4f)$	29252	24040±900	0.822±0.031	$G^1(5p,5d)$	41701	41701 (fix)
$G^2(5p,4f)$	22845	18855±720	0.825±0.032	$G^3(5p,5d)$	25951	25951 (fix)
$G^4(5p,4f)$	15446	9947±920	0.644±0.060	ζ_{5p}	6893	6893 (fix)
ζ_{5p}	6920	8421±190	1.217±0.027	ζ_{5d}	381	381 (fix)
ζ_{4f}	48	0±60	0.000±1.250			
$5f$				Configuration interaction integrals		
E_{av}		216345±180		$p-6p$		
$F^2(5p,5p)$	52207	41766 (fix)	0.800	$R^2(5p5p,5p6p)$	5419(.349) ^a	5419 (fix)
				$p-4f$		
				$R^2(5p5p,5p4f)$	-32918(-.940)	-32918 (fix)
				$p-5f$		
				$R^2(5p5p,5p5f)$	-20304(-.911)	-20304 (fix)
				$p-5d$		
				$R^1(5s5p,5p5d)$	51463(.998)	51463 (fix)
				$R^2(5s5p,5d5p)$	37121(.996)	37121 (fix)

$4p-p^6$				
$R^1(5s5s,5p5p)$	67375(1.000)	67375 (fix)	1.0	
6p-4f				
$R^2(5p6p,5p4f)$	3107(.197)	3107 (fix)	1.0	
$R^2(5p6p,4f5p)$	-2428(-.220)	-2428 (fix)	1.0	
6p-5f				
$R^2(5p6p,5p5f)$	-4503(-.530)	-4503 (fix)	1.0	
$R^2(5p6p,5f5p)$	2450(-.360)	2450 (fix)	1.0	
6p-5d				
$R^1(5s6p,5p5d)$	7831(.331)	7831 (fix)	1.0	
$R^2(5s6p,5d5p)$	-2443(-.199)	-2443 (fix)	1.0	
4f-5f				
$R^2(5p4f,5p5f)$	15068(.859)	8670±5160	0.575±0.340	
$R^2(5p4f,5f5p)$	13820(.896)	13159±1584	0.952±0.120	
$R^4(5p4f,5f5p)$	9564(.960)	9594 (fix)	1.0	
4f-5d				
$R^1(5s4f,5p5d)$	-37462(-.894)	-17636 (fix)	0.471	
$R^2(5s4f,5d5p)$	-24234(-.941)	-24234 (fix)	1.0	
5f-5d				
$R^1(5s5f,5p5d)$	-16823(-.720)	-7920 (fix)	0.471	
$R^2(5s5f,5d5p)$	-14589(-.910)	-14589 (fix)	1.0	
5d-p ⁶				
$R^1(5s5d,5p5p)$	50988(.998)	50988 (fix)	1.0	

^aThe values in parentheses are a measure of the amount of cancellation which occurred in forming the integral. These numbers are the ratio of the true R^k value to an R^k value calculated using the absolute value of each wavefunction.

Table VI. Comparison between observed and calculated energy-level values (in cm^{-1}) and calculated percentage compositions for the $5s5p^5 + 5s^25p^3(6s+7s+5d+6d)$ configurations of Xe III. Eigenvector components larger than 5% are given. Observed [3] and calculated g_J factors are listed

J	E(obs.)	E(calc.)	Obs.-Calc.	g_J (obs.)	g_J (calc.)	Percentage composition
5	132 160	132 443	-283		1.20	100 (2D)5d ³ G
	200 472	200 436	35		1.20	100 (2D)6d ³ G
4	112 272	112 250	21		1.47	88 (4S)5d ⁵ D + 10 (2P)5d ³ F
	127 782	127 735	47		1.16	40 (2D)5d ³ G + 27 (2D)5d ³ F + 16 (2P)5d ³ F + 9 (2D)5d ¹ G
	130 174	130 702	-528		1.20	71 (2D)5d ³ F + 22 (2D)5d ³ G
	132 712	132 800	-88		1.02	73 (2D)5d ¹ G + 25 (2D)5d ³ G
	148 536	148 459	76		1.21	70 (2P)5d ³ F + 13 (2D)5d ¹ G + 12 (2D)5d ³ G
	182 716	182 754	-37		1.46	85 (4S)6d ⁵ D + 12 (2P)6d ³ F
	196 538	196 411	127		1.13	42 (2D)6d ³ G + 31 (2D)6d ¹ G + 15 (2P)6d ³ F + 10 (4S)6d ⁵ D
	200 051	200 074	-24		1.06	43 (2D)6d ³ G + 42 (2D)6d ¹ G + 15 (2D)6d ³ F
	200 426	200 451	-25		1.21	82 (2D)6d ³ F + 16 (2D)6d ¹ G
3	111 605	111 401	204		1.44	80 (4S)5d ⁵ D + 6 (2P)5d ³ F + 6 (2P)5d ³ D
	121 230	121 363	-133		1.29	37 (4S)5d ³ D + 25 (2D)5d ³ D + 15 (4S)5d ⁵ D + 6 (2D)5d ³ G + 6 (2P)5d ³ F + 5 (2D)5d ³ F
	126 120	126 121	-1		1.12	58 (2D)5d ³ F + 11 (4S)5d ³ D + 11 (2D)5d ³ D + 10 (2P)5d ³ F + 8 (2D)5d ³ G
	128 349	128 386	-35		0.87	66 (2D)5d ³ G + 18 (2D)5d ³ F + 7 (4S)5d ⁵ D
	138 658	139 048	-389	1.33	1.33	83 (2D)6s ³ D + 8 (2D)5d ³ D
	143 156	143 110	46	1.22	1.22	38 (2D)5d ³ D + 21 (4S)5d ³ D + 12 (2P)5d ³ F + 10 (2D)5d ³ G + 7 (4S)5d ⁵ D + 6 (2D)6s ³ D
	145 341	145 259	83		1.14	56 (2P)5d ³ F + 11 (2P)5d ³ D + 7 (2D)6s ³ D + 6 (2D)5d ³ F + 6 (2D)5d ³ D + 5 (4S)5d ³ D
	148 413	148 691	-278		1.16	42 (2D)5d ¹ F + 31 (2P)5d ³ D + 10 (4S)5d ³ D
	156 393	156 261	132		1.15	33 (2P)5d ³ D + 32 (2P)5d ¹ F + 15 (2D)5d ¹ F + 6 (2D)5d ³ F + 5 (2D)5d ³ D
	162 958	163 174	-216		1.04	40 (2P)5d ¹ F + 35 (2D)5d ¹ F + 7 (2P)5d ³ D + 5 (4S)5d ³ D + 5 (2D)6d ¹ F
	182 464	182 430	34		1.44	79 (4S)6d ⁵ D + 6 (2P)6d ³ D + 6 (2P)6d ³ F
	186 384	186 311	74		1.28	71 (4S)6d ³ D + 9 (2P)6d ¹ F + 6 (4S)6d ⁵ D
	196 262	196 304	-42		0.93	58 (2D)6d ³ G + 11 (4S)6d ³ D + 11 (2D)6d ³ F + 8 (2P)6d ¹ F + 7 (2D)6d ³ D
	196 609	196 640	-31		1.13	43 (2D)6d ³ F + 13 (2D)6d ³ G + 11 (2D)6d ³ D + 9 (2P)6d ³ D + 9 (4S)6d ⁵ D + 6 (2D)6d ¹ F + 6 (2P)6d ³ F
	200 033	200 054	-21		1.33	99 (2D)7s ³ D
	200 650	200 815	-165		1.25	64 (2D)6d ³ D + 30 (2D)6d ³ F
	203 846	203 921	-76		1.04	71 (2D)6d ¹ F + 11 (2D)6d ³ D + 5 (2D)6d ³ G
	98 262	98 217	45		1.50	75 $p^5\ ^3P$ + 16 (2D)5d ³ P + 8 (2P)5d ³ P

111 856	111 593	264		1.40	$78 ({}^4S)5d^5D + 6 ({}^2P)5d^3D$
117 240	117 130	110		1.09	$27 ({}^4S)5d^3D + 17 ({}^2D)5d^3D + 16 ({}^2D)5d^3F + 15 ({}^4S)5d^5D + 12 ({}^2P)5d^1D + 6 ({}^2P)5d^3F$
121 476	121 343	133	1.95	1.93	$87 ({}^4S)6s^5S + 10 ({}^2P)6d^3P$
124 692	124 721	-30		0.86	$52 ({}^2D)5d^3F + 18 ({}^2D)5d^3D + 16 ({}^4S)5d^3D + 11 ({}^2P)5d^3F$
134 667	134 767	-99	1.18	1.20	$33 ({}^2D)6s^3D + 20 ({}^2D)6s^1D + 12 ({}^2P)5d^1D + 11 ({}^2P)6s^3P + 6 ({}^4S)6s^5S + 6 ({}^2D)5d^1D$
136 367	136 137	231	0.90	1.08	$22 ({}^2D)6s^3D + 16 ({}^2D)5d^3D + 15 ({}^2P)5d^1D + 15 ({}^2D)5d^1D + 10 ({}^2P)5d^3F + 8 ({}^2P)5d^3D$
142 064	141 824	241	1.12	1.17	$24 ({}^2D)5d^3D + 22 ({}^4S)5d^3D + 18 ({}^2P)5d^3D + 11 ({}^2D)6s^3D + 10 ({}^2P)5d^1D + 6 ({}^2P)6s^3P$
143 048	143 109	-61	0.96	1.02	$54 ({}^2D)6s^1D + 19 ({}^2D)6s^3D + 12 ({}^2P)5d^3F + 5 ({}^2P)5d^1D$
145 300	145 112	188	0.81	0.85	$50 ({}^2P)5d^3F + 18 ({}^2D)5d^3F + 13 ({}^2P)5d^3P + 8 ({}^2D)5d^1D$
148 370	148 590	-220		1.37	$39 ({}^2D)5d^3P + 14 p^5 {}^3P + 10 ({}^2P)5d^3P + 9 ({}^2D)5d^3D + 6 ({}^2P)5d^1D + 6 ({}^2P)5d^3D$
150 404	150 246	159		1.37	$54 ({}^2P)5d^3P + 12 ({}^2D)5d^3P + 6 ({}^2D)5d^1D + 5 ({}^2P)6s^3P$
153 893	153 614	279		1.22	$28 ({}^2P)5d^3D + 12 ({}^2D)5d^1D + 11 ({}^2D)5d^3P + 11 ({}^2P)6s^3P + 10 ({}^4S)5d^3D + 6 ({}^2P)5d^1D + 6 ({}^2D)5d^3D$
158 928	159 117	-189		1.41	$53 ({}^2P)6s^3P + 18 ({}^2D)5d^3P + 8 ({}^2D)6s^3D + 8 ({}^2D)6s^1D$
161 810	162 283	-473		1.04	$39 ({}^2D)5d^1D + 20 ({}^2P)5d^1D + 19 ({}^2P)5d^3D + 7 ({}^4S)5d^3D$
182 338	182 357	-19		1.66	$42 ({}^4S)6d^5D + 41 ({}^4S)7s^5S + 5 ({}^2P)7s^3P$
182 483	182 450	33		1.69	$45 ({}^4S)7s^5S + 38 ({}^4S)6d^5D + 6 ({}^2P)7s^3P$
185 121	185 220	-99		1.16	$62 ({}^4S)6d^3D + 10 ({}^2P)6d^1D + 6 ({}^2D)6d^3D + 6 ({}^4S)6d^5D$
195 977	195 970	7		0.95	$47 ({}^2D)6d^3F + 11 ({}^2D)7s^3D + 7 ({}^4S)6d^3D + 7 ({}^2D)6d^1D$
196 141	196 103	38		1.16	$38 ({}^2D)7s^3D + 20 ({}^2D)7s^1D + 13 ({}^2D)6d^3F + 13 ({}^2P)7s^3P + 7 ({}^4S)7s^5S$
198 492	198 506	-14		1.26	$37 ({}^2D)6d^3D + 22 ({}^2D)6d^3P + 9 ({}^2P)6d^3P$
200 540	200 520	20		1.06	$64 ({}^2D)7s^1D + 34 ({}^2D)7s^3D$
201 512	201 507	5		1.22	$44 ({}^2D)6d^3D + 30 ({}^2D)6d^3P + 13 ({}^2D)6d^1D + 6 ({}^2D)6d^3F$
203 376	203 194	183		1.13	$54 ({}^2D)6d^1D + 30 ({}^2D)6d^3P + 7 ({}^2D)6d^3F$
1 103 568	103 639	-71		1.45	$62 p^5 {}^3P + 14 ({}^2D)5d^3P + 8 ({}^2P)5d^3P$
112 450	112 328	122		1.48	$87 ({}^4S)5d^5D + 6 p^5 {}^3P$
119 026	118 935	91		1.01	$44 ({}^2D)5d^1P + 28 p^5 {}^1P + 7 ({}^2P)5d^1P + 7 p^5 {}^3P + 6 ({}^4S)5d^3D$
121 923	122 282	-359		0.60	$51 ({}^4S)5d^3D + 31 ({}^2D)5d^3D + 5 ({}^2P)5d^3D$
125 617	125 594	23	1.77	1.80	$78 ({}^4S)6s^3S + 7 ({}^2P)6s^1P$
133 234	133 412	-178	0.38	0.65	$36 ({}^2D)5d^3D + 25 ({}^2D)6s^3D + 22 ({}^2P)5d^3D + 6 ({}^4S)6s^3S$
138 145	138 128	17	0.50	0.70	$49 ({}^2D)6s^3D + 17 ({}^2D)5d^3D + 9 ({}^2P)5d^3D + 6 ({}^2P)6s^1P + 6 ({}^4S)6s^3S + 5 ({}^4S)5d^3D$
140 731	140 464	267		1.53	$44 ({}^2P)5d^3P + 19 ({}^2D)5d^3S + 18 ({}^2D)5d^3P$
147 798	147 630	168		1.70	$49 ({}^2D)5d^3S + 20 ({}^2P)6s^3P + 18 ({}^2D)5d^3P$
151 482	151 584	-102	1.47	1.46	$46 ({}^2P)6s^3P + 22 ({}^2P)6s^1P + 15 ({}^2D)5d^3S + 12 ({}^2P)5d^3P$
154 639	154 546	93		1.30	$20 ({}^2D)5d^3P + 18 p^5 {}^1P + 15 ({}^2P)5d^3P + 13 ({}^2P)6s^1P + 9 ({}^2D)5d^3S +$

				$7 p^5 3p + 7 ({}^2D)5d^1p$
155 401	155 333	68	0.64	$45 ({}^2P)5d^3D + 16 ({}^4S)5d^3D + 12 ({}^2P)5d^1p + 8 ({}^2D)5d^3D + 6 ({}^4S)6d^3D$
159 388	159 126	262	1.20	$32 ({}^2P)6s^1p + 20 ({}^2P)6s^3p + 14 ({}^2D)5d^3p + 13 ({}^2D)6s^3D + 6 p^5 3p + 6 ({}^2P)5d^3p$
163 527	163 844	-316	0.99	$33 ({}^2D)5d^1p + 27 p^5 1p + 10 ({}^2P)6s^1p + 7 ({}^2P)5d^3D + 7 ({}^2P)5d^3p$
175 050	174 482	568	0.99	$64 ({}^2P)5d^1p + 8 p^5 1p + 6 ({}^2P)6d^1p + 5 ({}^4S)5d^3D$
182 551	182 496	55	1.45	$85 ({}^4S)6d^5D + 8 ({}^2P)6d^3p$
183 786	183 795	-9	1.84	$84 ({}^4S)7s^3S + 8 ({}^2P)7s^1p$
186 589	186 645	-56	0.60	$76 ({}^4S)6d^3D + 5 ({}^2P)6d^3D + 5 ({}^2P)6d^1p$
195 907	195 948	-41	0.77	$57 ({}^2D)7s^3D + 11 ({}^2D)6d^3D + 8 ({}^4S)7s^3S + 7 ({}^2P)7s^1p$
196 877	196 881	-5	0.74	$45 ({}^2D)6d^3D + 18 ({}^2D)7s^3D + 12 ({}^2D)6d^1p$
199 104	199 122	-18	1.58	$45 ({}^2D)6d^3S + 21 ({}^2D)6d^3p + 10 ({}^2P)6d^3p + 7 ({}^2D)6d^1p$
202 036	202 066	-31	1.16	$46 ({}^2D)6d^3p + 22 ({}^2D)6d^1p + 22 ({}^2D)6d^3D$
202 806	202 589	217	1.45	$38 ({}^2D)6d^3S + 37 ({}^2D)6d^1p + 16 ({}^2D)6d^3p$
0	108 334	108 380	-46	$55 p^5 3p + 22 ({}^4S)5d^5D + 12 ({}^2D)5d^3p$
	112 694	112 591	103	$69 ({}^4S)5d^5D + 20 p^5 3p + 9 ({}^2D)5d^3p$
		126 871		$85 ({}^2D)5d^1s + 8 ({}^2P)5d^3p$
140 438	140 556	-118		$42 ({}^2P)5d^3p + 31 ({}^2D)5d^3p + 12 ({}^2D)5d^1s + 8 ({}^2P)6s^3p$
150 505	150 324	181		$87 ({}^2P)6s^3p + 10 ({}^2P)5d^3p$
160 734	160 743	-9		$43 ({}^2D)5d^3p + 28 ({}^2P)5d^3p + 20 p^5 3p$
182 522	182 482	40		$86 ({}^4S)6d^5D + 11 ({}^2P)6d^3p$
197 091	197 024	67		$58 ({}^2D)6d^1s + 19 ({}^2D)6d^3p + 15 ({}^2P)6d^3p + 8 ({}^4S)6d^5D$
201 618	201 847	-228		$62 ({}^2D)6d^3p + 32 ({}^2D)6d^1s$

Mean error of the least-squares fit $\sigma = [\sum (E_{\text{obs}} - E_{\text{calc}})^2 / (N-P)]^{1/2} = 217 \text{ cm}^{-1}$ with $N=83$ known and $P=30$ adjustable parameters

Table VII. Energy parameters (in cm⁻¹) for the 5s5p⁵5s²5p³(5d+6d+6s+7s) configurations of Xe III

Parameter	HF(E _{av})	Fitted	Fitted/HF
p⁵			
E _{av}		123209±430	
G ¹ (5s,5p)	67295	47314±950	0.703±0.014
ζ _{5p}	6605	7760±310	1.175±0.047
6s			
E _{av}		140786±90	
F ² (5p,5p)	52231	41089±630	0.787±0.012
G ¹ (5p,6s)	4544	3795±250	0.835±0.055
ζ _{5p}	7169	8078±190	1.127±0.027
7s			
E _{av}		200200±160	
F ² (5p,5p)	52644	40033±1320	0.760±0.025
G ¹ (5p,7s)	1376	1072±300	0.779±0.220
ζ _{5p}	7261	8072±490	1.112±0.360
5d			
E _{av}		136928±130	
F ² (5p,5p)	51522	39438±440	0.765±0.009
F ² (5p,5d)	35641	29232±440	0.820±0.012
G ¹ (5p,5d)	40265	28868±570	0.717±0.014
G ³ (5p,5d)	25050	16810±560	0.671±0.022
ζ _{5p}	6933	8308±100	1.198±0.014
ζ _{5d}	358	467±60	1.304±0.170

6d					
E _{av}	200589±140				
F ² (5p,5p)	52621	40006±630	0.760±0.012		
F ² (5p,6d)	8853	6757±820	0.763±0.093		
G ¹ (5p,6d)	6482	2384±580	0.368±0.089		
G ³ (5p,6d)	4400	1089±710	0.248±0.160		
ζ _{5p}	7239	8456±240	1.168±0.033		
ζ _{6d}	98	161±52	1.643±0.530		
Configuration interaction integrals					
p⁵-6s					
R ¹ (5p5p,5s6s)		375(.014) ^a	375 (fix)	1.0	
p⁵-7s					
R ¹ (5p5p,5s7s)		-318(-.021)	-318 (fix)	1.0	
p⁵-5d					
R ¹ (5p5p,5s5d)		50086(.998)	33048±300	0.660±0.006	
p⁵-6d					
R ¹ (5p5p,5s6d)		20212(.919)	16016±1760	0.792±0.087	
6s-7s					
R ¹ (5p6s,7s5p)		2426(.370)	2426 (fix)	1.0	
6s-5d					
R ² (5p6s,5p5d)		-9991(-.507)	-9991 (fix)	1.0	
R ¹ (5p6s,5d5p)		-2966(-.141)	-2966 (fix)	1.0	
6s-6d					
R ² (5p6s,5p6d)		3214(-.379)	3214 (fix)	1.0	
R ¹ (5p6s,6d5p)		271(-.031)	271 (fix)	1.0	

7s-5d				
$R^2(5p7s, 5p5d)$	-4994(-.453)	-4994 (fix)	1.0	
$R^1(5p7s, 5d5p)$	-2042(-.167)	-2042 (fix)	1.0	
7s-6d				
$R^2(5p7s, 5p6d)$	-2138(-.384)	-2138 (fix)	1.0	
$R^1(5p7s, 6d5p)$	-148(-.029)	-148 (fix)	1.0	
5d-6d				
$R^2(5p5d, 5p6d)$	11112(.756)	11638±1720	1.047±0.160	
$R^1(5p5d, 6d5p)$	15402(.901)	14647±1150	0.951±0.075	
$R^3(5p5d, 6d5p)$	9957(.943)	5000 (fix)	0.502	

^a The values in parentheses are a measure of the amount of cancellation which occurred in forming the integral. These numbers are the ratio of the true R^k value to an R^k value calculated using the absolute value of each wavefunction.

Table VIII.

Comparison between xenon $N_{4,5}^{00}$ Auger spectrum and optical spectrum of Xe^{2+}

Optical data: Present work

Auger data : L.O. Werme, T. Bergmark, K. Siegbahn [19]

Auger data				Optical data		Energy difference cm ⁻¹ (Optical-Auger)
Line no	Intensity	Energy		Classification	%5s5p ⁵	
		eV	cm ⁻¹		1 _p	3 _p
1,3	15,86	0	0	5s ² 5p ⁴ 3 _p ₂		0
2,6	43,39	1.21	9759	3 _p ₁		+35
-,5	-,48	1.00	8065	3 _p ₀		+65
4,7	104,97	2.12	17098	1 _D ₂		+1
8,9	100,73	4.49	36214	1 _S ₀		-111
13,15	11,7	12.17	98157	5s5p ⁵ 3 _p ₂	- 75	+106
14,-	10,-	12.85	103642	3 _p ₁	5 62	-74
16,18	62,80	14.76	119047	(² D)5d 1 _p ₁	28 7	-21
17,19	3,8	15.13	121991	(⁴ S)5d 3 _D ₁	2 1	-68
20,23	7,11	17.44	140703	(² P)5d 3 _p ₁	2 -	+28
22,25	41,74	19.17	154615	(² D)5d 3 _p ₁	18 7	+24
-,26 ^a	-,31	19.73	159133	(² P)6s 1 _p ₁	1 6	+256
24,27	90,134	20.27	163488	5s5p ⁵ 1 _p ₁	27 2	+40
26,28	31,25	21.70	174981	(² P)5d 1 _p ₁	8 1	+72
29,30	107,133	26.13	210751	5s ⁰ 5p ⁶ 1 _S ₀		+106

^aDoubly classified

PAPER IV

NATURAL RADIATIVE LIFETIMES AND HYPERFINE STRUCTURE OF THE $4s^2 6p \ ^2P_{3/2,1/2}$ LEVELS OF GALLIUM

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Natural radiative lifetimes and the signs of previously determined hyperfine coupling constants were determined for the $4s^2 6p \ ^2P_{3/2,1/2}$ levels of gallium. The lifetimes were found to be 167(4) and 172(9) ns, respectively. In addition, the quadrupole moments of ^{69}Ga [0.17(3) b] and ^{71}Ga [0.10(2) b] were deduced, and the isotope shifts in the 639.7 and 641.3 nm Ga lines were determined.

Gallium is a group-three element with ground configuration $4s^2 4p$. On excitation of the outer 4p electron, an alkali-like spectrum is produced. However, the ground state is a $^2P_{1/2}$ state. The hyperfine coupling constants of this state and its metastable fine-structure partner $4p \ ^2P_{3/2}$ were measured with high precision using atomic-beam magnetic-resonance spectroscopy [1]. In a theoretical analysis by Bessis et al. [2], the importance of polarization and relativistic effects are shown. Comparatively few excited states have been investigated in gallium. The hfs of the first excited $^2S_{1/2}$ state, 5s, was recently determined by Neijzen and Dönszelmann [3]. These authors have also performed a quantum-beat experiment on the $6p \ ^2P_{3/2,1/2}$ states [4], yielding the magnetic-dipole and the electric quadrupole coupling constants a and b of the two stable spin 3/2 isotopes ^{69}Ga (60%) and ^{71}Ga (40%) with high precision. However, the signs of the interaction constants cannot be determined in such experiments. In the present paper we report the results of a high-resolution study of the 639.7 nm ($5s \ ^2S_{1/2} - 6p \ ^2P_{3/2}$) and 641.3 nm ($5s \ ^2S_{1/2} - 6p \ ^2P_{1/2}$) gallium lines yielding these signs and, in addition, the optical isotope shifts in these lines. A multi-mode and a single-mode dye laser were used for step-wise excitation of a collimated atomic beam. By pulse-modulating the second-step laser acousto-optically, the natural lifetimes of the P states, previously known only with low precision [4], were determined in delayed-coincidence experiments.

The experimental set-up used in the high-resolution experiments is similar to the one used in recent investigations on In [5] and Al [6] in our laboratory. The principles for the special kind of delayed-coincidence we used (PUMOLS) can be found in ref. [7] and the experimental arrangement is similar to the one used in ref. [8].

In fig. 1 a recording of the 641.3 nm line is shown together with an excitation scheme and a hyperfine-transition diagram. From the relative intensities of the hyperfine components it is evident that the a factors are positive in the $^2P_{1/2}$ and the $^2S_{1/2}$ states for both isotopes. However, because of line broadening due to the short-lived intermediate S-state ($\tau \approx 6$ ns [9]) and residual Doppler effect, the deduced a factors are less precise than, although consistent with, the results given by Neijzen and Dönszelmann ($|a_{1/2}(71)| = 67.4(7)$ MHz; $|a_{1/2}(69)| = 53.3(7)$ MHz; $|a_{5s}(71)| = 2716.0(30)$ MHz; $|a_{5s}(69)| = 2137.7(20)$ MHz for ^{69}Ga and ^{71}Ga) [3,4].

For the even less resolved 639.7 nm line, a computer program, generating a resulting overlapped structure from a given set of interaction constants and a chosen experimental linewidth, was used for establishing that the a and b factors for the $6p \ ^2P_{3/2}$ state given in ref. [4] ($|a_{3/2}(71)| = 28.5(2)$ MHz; $|b_{3/2}(71)| = 2.4(3)$ MHz; $|a_{3/2}(69)| = 22.4(2)$ MHz; $|b_{3/2}(69)| = 3.2(3)$ MHz) are positive for both isotopes. (The quantum-beat experiment establishes that the a and b factors have the same signs.) From a large number of experi-

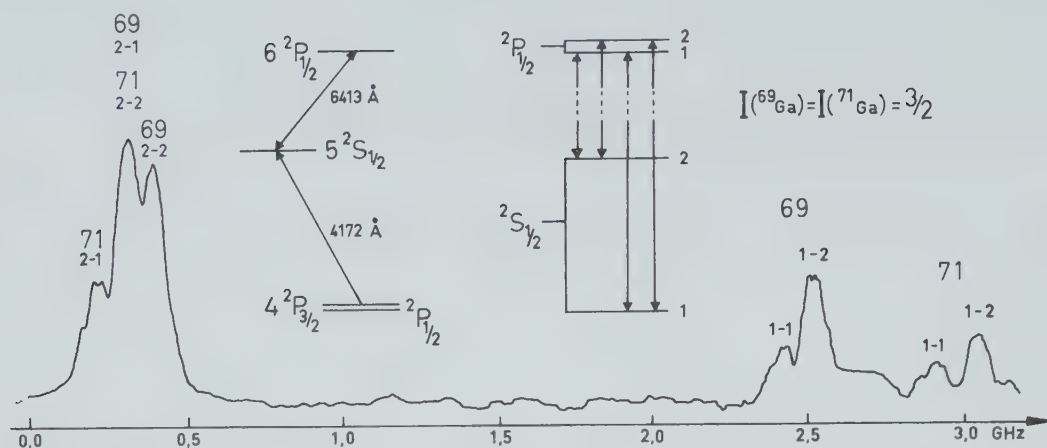


Fig. 1. Experimental recording of the 641.3 nm Ga line ($5^2S_{1/2}-6^2P_{1/2}$) and diagrams illustrating the step-wise excitation scheme and hyperfine transitions.

mental curves, the isotope shifts $\Delta\nu(71-69)$ were also determined, employing the coupling-constant results of refs. [3,4]. We find $\Delta\nu(71-69) = 149(8)$ MHz for the 641.3 nm line and $\Delta\nu(71-69) = 143(8)$ MHz for the 639.7 nm line. The error bars are determined by the experimental scattering and the estimated uncertainty in the used deconvolution procedure. The cor-

responding normal mass shifts (nms) are 105 MHz for both lines. The specific mass shift (sms) for an S-P transition is estimated by Heilig and Steudel [10] as $\Delta\nu(\text{sms}) = (0.3 \pm 0.9) \Delta\nu(\text{nms})$ or 31 ± 94 MHz in our case. This leaves 13 and 7 MHz with large uncertainties for the field shift of the 641.3 and 639.7 nm lines, respectively.

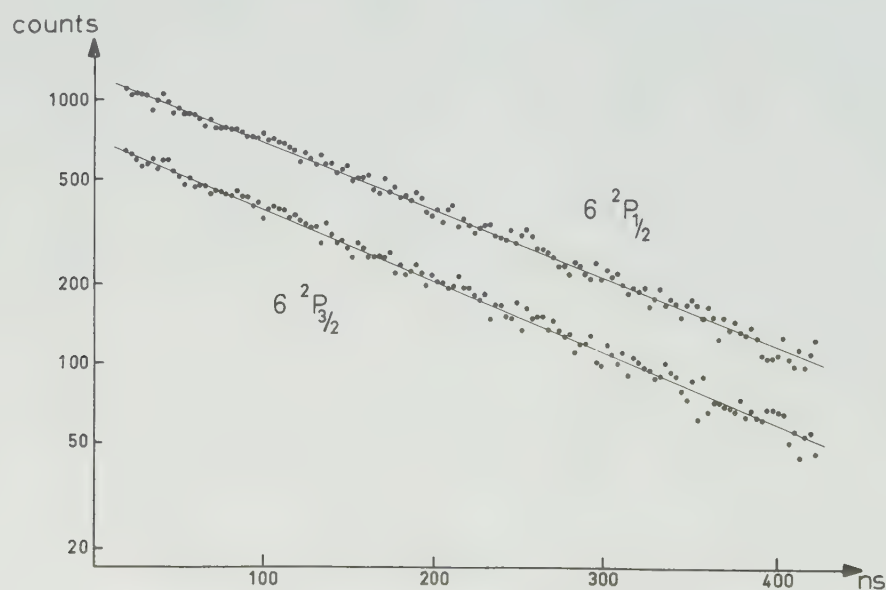


Fig. 2. Experimental decay curves shown on a logarithmic scale. The background (about 50 counts) has been subtracted. Exponential fits to the data are included.

Table 1

Results for ^{69}Ga . One-electron expressions from ref. [13] have been used with the following parameters: $F_T(1/2) = 1.0757$, $F_T(3/2) = 1.0154$, $H_T = 1.0174$, $R_T = 1.0314$, $Z_i = 27$. Experimental values are from refs. [1,4].

State	$a_{3/2}$ (MHz)	$a_{3/2,\text{corr}}$ (MHz)	$\langle a_0^3/r^3 \rangle$ from $a_{3/2,\text{corr}}$	$\langle a_0^3/r^3 \rangle$ from δW	b (MHz)	Q (barn)
$6p^2P_{3/2}$	22.4(2)	12.0	0.164	0.171	3.2(3)	0.197
$4p^2P_{3/2}$	190.79428(15)	242.9	3.33	3.43	62.52247(30)	0.191

In our lifetime measurements the red laser was pulse-modulated acousto-optically. A sufficiently high magnetic field was applied to prevent Zeeman quantum beats due to the earth's magnetic field to influence the results. In fig. 2 examples of experimental curves with fitted exponentials are shown on a logarithmic scale. We obtain $\tau(6p^2P_{1/2}) = 172(9)$ ns and $\tau(6p^2P_{3/2}) = 167(4)$ ns in agreement with ref. [4] [160(35) ns and 150(15) ns, respectively], but considerably more precise. Our error bars are determined from the statistical scattering of data and with consideration of possible systematic effects.

We will finish this paper with a simple analysis of the discussed hyperfine structure, based on the assumption that the radial parameters for the orbital and the spin-dipole interactions are equal. The procedure reviewed in ref. [11] and applied for alkali-atom P states, e.g. in ref. [12] was shown to apply remarkably well to In P states [5]. In this semi-empirical approach, the effect of core polarization a_c can be isolated and corrected a factors, referring to the p-electron alone can be calculated. In table 1 the results of this calculation of the radial parameters for the 4p and 6p states are given for ^{69}Ga together with values derived from the observed fine structure δW using simple one-electron expressions [13]. It can be seen that the core polarization is quite significant and of different sign for the 4p and 6p states. Quite consistent results are obtained from the fine and hyperfine structure. Using the mean value for the radial parameter together with the experimental b factors, the quadrupole moment Q for ^{69}Ga is also calculated to be 0.197 b and 0.191 b from the 6p and 4p states, respectively. Corresponding Q -values for ^{71}Ga are 0.117 b and 0.120 b. The values are remarkably consistent. Using the Sternheimer correcting factor 0.886 [14], calculated for the 4p state also for the 6p state, we obtain as "best" values for the quadrupole

moments $Q(^{69}\text{Ga}) = 0.17(3)$ b and $Q(^{71}\text{Ga}) = 0.10(2)$ b. Here the error bars are mainly determined by the estimated uncertainty in the used evaluation procedure. For obtaining more accurate results, a many-body calculation [15] should be performed.

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References

- [1] R.T. Daly and J.H. Holloway, Phys. Rev. 96 (1954) 539; A. Lurio and A.G. Prodell, Phys. Rev. 101 (1956) 79.
- [2] N. Bessis, J. Picart and J.P. Desclaux, Phys. Rev. 187 (1969) 88.
- [3] J.H.M. Neijzen and A. Dönszelmann, Physica 98C (1981) 235.
- [4] J.H.M. Neijzen and A. Dönszelmann, submitted to Physica C.
- [5] Jiang Zhan-Kui, H. Lundberg and S. Svanberg, Z. Phys. A306 (1982) 7.
- [6] Jiang Zhan-Kui, H. Lundberg and S. Svanberg, Phys. Lett. 92A (1982) 27.
- [7] M. Gustavsson, H. Lundberg, L. Nilsson and S. Svanberg, J. Opt. Soc. Am. 69 (1979) 984.
- [8] A. Aymar, P. Grafström, C. Levinson, H. Lundberg and S. Svanberg, J. Phys. B15 (1982) 877.
- [9] A. Lindgård, S. Mannervik, B. Jelenković and E. Veje, Z. Phys. A301 (1981) 1.
- [10] K. Heilig and A. Steudel, At. Data Nucl. Data Tables 14 (1974) 613.
- [11] W. Fischer, Fortschr. Phys. 18 (1970) 89.
- [12] G. Belin and S. Svanberg, Phys. Scr. 4 (1971) 269.
- [13] H. Kopfermann, Nuclear moments (Academic Press, New York, 1958).
- [14] R.M. Sternheimer, Phys. Rev. A6 (1972) 1702.
- [15] I. Lindgren and J. Morrison, Atomic many-body theory, Springer series in chemical physics, Vol. 13 (Springer, Berlin, 1982); P. Grundevik, H. Lundberg, A.-M. Mårtensson, K. Nyström and S. Svanberg, J. Phys. B12 (1979) 2645.

PAPER V

Experimental and Theoretical Studies of the $4s^2 n p^2 P$ Sequence in Neutral Gallium

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Using time-resolved laser spectroscopy lifetime values as well as hyperfine coupling constants have been determined for the $4s^2 n p^2 P_{3/2}$ ($n=7-11$) states in ^{69}Ga and ^{71}Ga . Theoretical calculations of hyperfine structures based on many-body perturbation theory have been performed in the same sequence ($n=4-8$) for both fine-structure components. The theoretical values are compared with existing experimental data.

PACS: 31.30. Gs; 32.70. Fw; 35.10. Fk

Introduction

During recent years, groups in Lund and Amsterdam have been studying the group IIIA elements Al, Ga and In, using laser spectroscopy techniques. A large number of lifetime values have been determined using time-resolved techniques [1–3]. High resolution techniques employing cw lasers have been used to determine hyperfine structures (hfs) and isotope shifts in lower-lying states [4–6]. With the quantum beat method small hfs splittings in higher-lying states have also been determined [7–9]. Calculations using many-body perturbation theory (MBPT) [10] have given values for the magnetic dipole constant of low-lying states [11]. However, since correlation effects were not included in these calculations large deviations from experimental data were found. In this paper we present new experimental data concerning lifetimes and hfs in the $4s^2 n p^2 P$ sequence ($n=7-11$, $J=3/2$) in gallium. Extended MBPT calculations for both fine-structure components in this sequence ($n=4-8$) have been performed, including core polarization, correlation and relativistic effects.

Experimental Arrangements

The experimental set-up is shown in Fig. 1. Two dye lasers pumped by an excimer laser (Lambda Physik

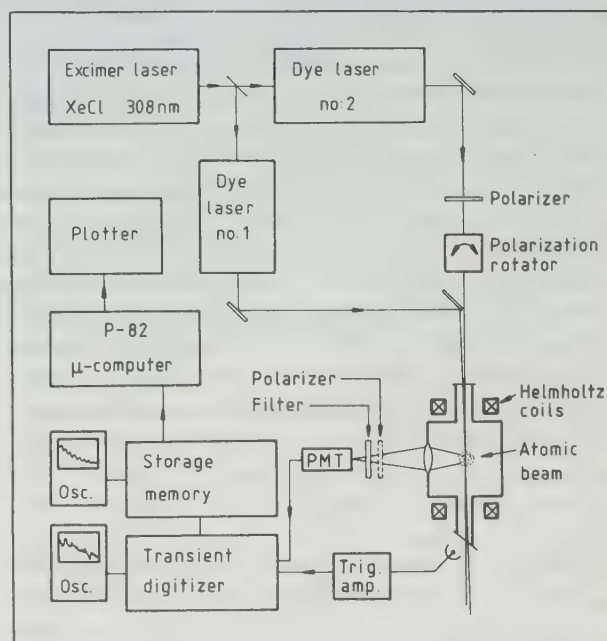


Fig. 1. Experimental set-up for lifetime and quantum beat measurements on $^{69,71}\text{Ga}$

EMG 102E with XeCl gas) were used for step-wise excitation. A home-built Littman cavity dye laser, operating on Stilbene 1, was used to populate the $4s^2 5s^2 S_{1/2}$ intermediate level (417.2 nm). About 90% of the excimer light was used to pump the second step laser (Lambda Physik FL 2002) which was

operated on Coumarin 47 or Coumarin 307 dye. The two dye laser beams were temporally and spatially overlapped in an atomic beam of gallium. The polarization angle of the second step laser could be set with a polarization rotator. The magnetic field in the excitation region was controlled by Helmholtz coils. The fluorescence light from an excited state passed through appropriate filters and was imaged on a fast photomultiplier tube (EMI 9816 QB). During the quantum beat measurements a plane polarizer was inserted on the detection side. Signals coming from the photomultiplier tube were captured by a transient recorder (Biomation 8100) and added in a storage memory. Typically 1,000 transients were collected before a recording was transferred to a P-82 microcomputer for evaluation.

Measurements and Results

A schematic energy level diagram is shown in Fig. 2. The wavelength settings of the second-step laser could be found in the literature [12] except for the $4s^28p^2P_{1/2, 3/2}$ states. The air wavelengths for these states were 493.95(5) and 493.71(5) nm, respectively, when taken from the dye laser setting.

The lifetime measurements were performed on a low-density atomic beam in order to avoid multiple scattering and nonradiative decay via collisions. A fairly large magnetic field (~ 5 mT) eliminated distortion of the decay curves due to slow Zeeman quantum beats. The lifetime values of both $4s^2np^2P_{1/2, 3/2}$ fine-structure components were measured separately but no significant difference was found. In Table 1 lifetime values of the doublets are given. Lifetime values in a hydrogen-like sequence are expected to follow a $(n^*)^3$ dependence, where n^* is the effective principal quantum number. In this case we found

$$\tau = 6.0 \cdot (n^*)^{2.67}; \quad (n = 7-11).$$

However, it should be noted that long-lived states are vulnerable to transitions induced by black-body radiation [13, 14] and that the stated values refer to room temperature.

During the quantum beat measurements of the hyperfine structure the Earth's magnetic field was compensated for. The current through the compensating coils was determined using Zeeman quantum beats in the $6s6p^3P_1 - 6s^21S_0$ transition in ytterbium. The two isotopes of gallium, ^{69}Ga and ^{71}Ga , have natural abundances of 60% and 40%, respectively, and both have a nuclear spin of $I=3/2$. With right-angle geometry (between the atomic beam, excitation and

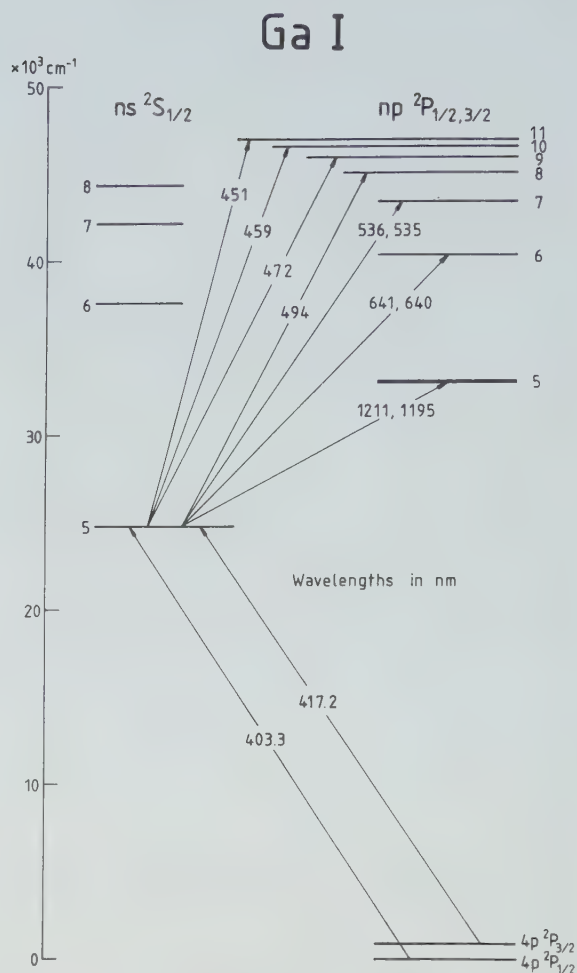


Fig. 2. Energy level diagram of neutral gallium

Table 1. Observed lifetimes

n	Lifetimes (ns)
7	380 ± 20
8	660 ± 40
9	920 ± 60
10	$1,450 \pm 100$
11	$2,000 \pm 200$

detection), only the $J=3/2$ fine structure component in the $4s^2np^2P$ sequence will cause beats [15]. The selection rules for hyperfine quantum beats are $\Delta F = 1, 2$. If the splittings in the $4s^2np^2P_{3/2}$ states are expressed in terms of the magnetic dipole constant, A , and the electric quadrupole constant, B , two sets of beat frequencies corresponding to $5A$, $3A+B$, $3A-2B$, $2A-B$ and $A-B$ are possible. A maximum beat amplitude is obtained when the polarizers for the excitation and detection light are parallel. In order to find as many as possible of the ten beat frequencies the following procedure was used. To

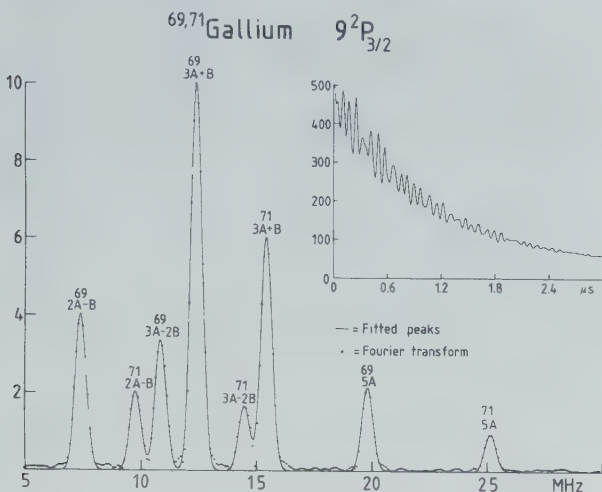


Fig. 3. Fluorescence decay and Fourier transform of the $9^2P_{3/2}$ state. The intensities on the vertical axes are given in arbitrary units

each recorded curve an exponential function, on a background, was fitted. The experimental curve was then divided by the exponential leaving an undamped beat structure. The divided curve was centred around zero and multiplied by an apodization function. Since the time spectrum is cut off, the peaks in the Fourier transformed spectrum will always have side-lobes. An apodization function can suppress these extra peaks at the price of somewhat broader lines. A number of apodization functions [16] were tested and a so-called Hamming window was used in our evaluation. The apodized curve was transformed into the frequency domain using a Fast Fourier Transform [16]. The peak positions were calculated from the amplitude spectrum by repeatedly fitting a gaussian curve to the highest peak and subtracting it from the spectrum. In this way we could determine eight of the ten possible lines. The intensity of the two $A-B$ peaks was too weak for the peaks to be identified. Figure 3 shows an experimental curve and the corresponding frequency spectrum. From the peak positions values of A and B were calculated using a multiple regression analysis program. The experimental A and B constants are given in Table 2. The experimental data for $n=7-11$ have a behaviour very close to an $(n^*)^{-3}$ dependence

$$\begin{aligned} A_{3/2}(69) &= 1,036.3 \cdot (n^*)^{-2.921} \text{ MHz} \\ A_{3/2}(71) &= 1,328.6 \cdot (n^*)^{-2.926} \text{ MHz} \\ B_{3/2}(69) &= 180.4 \cdot (n^*)^{-3.076} \text{ MHz} \\ B_{3/2}(71) &= 111.5 \cdot (n^*)^{-3.075} \text{ MHz.} \end{aligned}$$

This yields $\frac{\mu_{71}}{\mu_{69}} = 1.282$ and $\frac{Q_{71}}{Q_{69}} = 0.618$ which is in good agreement with $\frac{\mu_{71}}{\mu_{69}} = 1.270$ and $\frac{Q_{71}}{Q_{69}} = 0.629$ [17].

Table 2. Measured hyperfine constants

n	A (MHz)	B (MHz)
^{69}Ga		
7	11.13 ± 0.02	1.52 ± 0.03
8	6.35 ± 0.02	0.85 ± 0.01
9	3.96 ± 0.01	0.51 ± 0.02
10	2.64 ± 0.01	0.34 ± 0.01
11	1.84 ± 0.01	0.22 ± 0.02
^{71}Ga		
7	14.12 ± 0.03	0.95 ± 0.05
8	8.07 ± 0.02	0.52 ± 0.02
9	5.03 ± 0.01	0.31 ± 0.01
10	3.35 ± 0.01	0.21 ± 0.01
11	2.33 ± 0.01	0.13 ± 0.02

Theoretical Calculation of the Hyperfine Structure Using Many-Body Perturbation Theory

For the analysis of experimental hyperfine data as well as for the ab-initio evaluation of the hyperfine interaction (hfi) it is convenient to use the effective-operator formalism [18]. For an atomic system with an np configuration (outside closed shells) the magnetic dipole and electric quadrupole interaction constants can then be expressed

$$A(^2P_{1/2}) = C \cdot g_I \cdot \{4/3 \langle r^{-3} \rangle_{01} + 4/3 \langle r^{-3} \rangle_{12} - 1/3 \langle r^{-3} \rangle_{10}\} \quad (1a)$$

$$A(^2P_{3/2}) = C \cdot g_I \cdot \{2/3 \langle r^{-3} \rangle_{01} - 2/15 \langle r^{-3} \rangle_{12} + 1/3 \langle r^{-3} \rangle_{10}\} \quad (1b)$$

$$B(^2P_{1/2}) \equiv 0$$

$$B(^2P_{3/2}) = D \cdot Q \cdot 2/5 \cdot \langle r^{-3} \rangle_{02}.$$

Here, the parameters $\langle r^{-3} \rangle_{ij}$ correspond to the effective hyperfine parameters of rank i, j in spin and orbital space respectively (01=orbital, 12=spin-dipole, 10=contact and 02=quadrupole). g_I is the nuclear magnetic g factor and Q is the quadrupole moment of the nucleus. If the hyperfine constants are measured in MHz and the nuclear moments in nuclear magnetons (n.m.) and barns, then the constants C and D have the following values for ^{69}Ga

$$\begin{aligned} C &= 95.40943 \text{ MHz/n.m.} \\ D &= 234.9730 \text{ MHz/barn} \end{aligned}$$

using the values $\mu_{69} = +2.011 \text{ n.m.}$ and $Q_{69} = 0.178 \text{ barns}$ [17].

The effective hyperfine parameters can be given a well-defined interpretation by means of many-body perturbation theory (MBPT), and a particularly simple representation when the diagrammatic form of

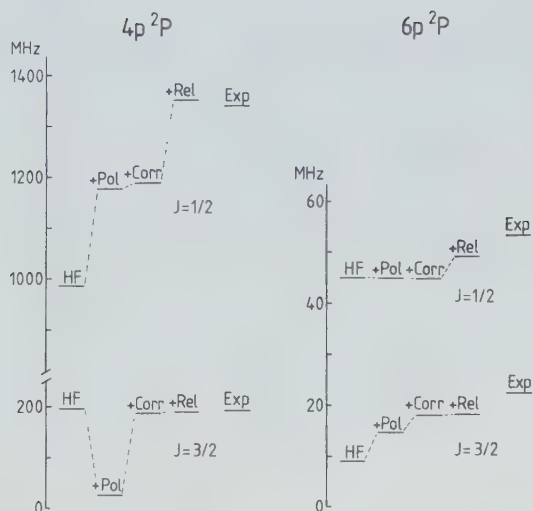


Fig. 4. Different contributions to the theoretical dipole-coupling constants. Illustrated by two of the investigated 2P states

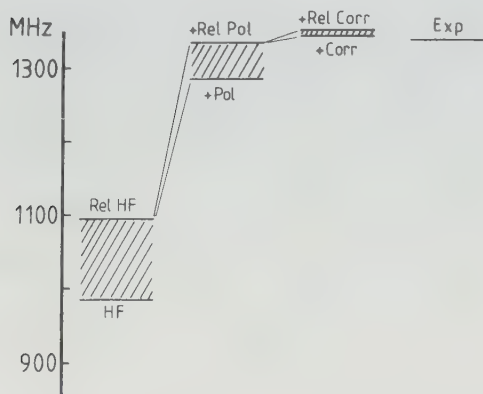


Fig. 5. Illustration of how relativistic effects add to the different contributions. Shown for the magnetic dipole-coupling constant for the $4p^2P_{1/2}$ ground state

this theory is used. In the present work we have used the form of MBPT developed, in particular, by the Chalmers group [10] to evaluate the hyperfine interaction for the $4s^2np$ states of gallium with $n = 4-8$. This procedure, which is based upon the numerical solution of inhomogeneous one- and two-particle equations, has been described in detail in the literature, and therefore we restrict ourselves here to a brief description of its main features.

The starting point for our calculations is with the non-relativistic Hartree-Fock (HF) functions, generated in the electron core of the singly ionized system (with the np electron removed), which we refer to as "HF $^{-1}$ ". The remaining interaction, i.e. the electron-electron interaction not included in HF $^{-1}$ and the hyperfine interaction, is then treated by means of perturbation theory. (For the moment we disregard

spin-orbit coupling and other relativistic effects.) The effect of the perturbation is to mix other (virtually excited) HF states with the HF state under consideration. These effects can be separated into one-, two-, ... body types, depending on the maximum number of electrons involved simultaneously in the "excitation". The one-body (single-particle) effects correspond to polarization of the core due to the interaction with the valence electron, and the polarized core interacts with the nucleus, leading to a hyperfine contribution. (Alternatively, the same effect can be regarded as a polarization, due to the nuclear moments, which interacts with the valence electron.) For core s electrons this effect is the important spin polarization, which leads to an induced contact interaction, also for non- s valence electrons ($\langle r^{-3} \rangle_{10}$ in (1)). Non- s electrons of the core also contribute to the polarization and affect the magnetic dipole as well as the electric quadrupole interaction – the latter effect usually being referred to as the Sternheimer effect [19].

In the present work the polarization effect is evaluated to all orders of perturbation theory by solving a set of inhomogeneous single-particle equations iteratively – a procedure which is essentially equivalent to unrestricted Hartree-Fock [20].

Two-particle- or pair-correlation effects can similarly be evaluated by solving inhomogeneous two-particle (pair) equations [21]. In the present work the pair functions are evaluated to first order, and by combining first-order single-particle and pair functions all third-order hyperfine effects can be evaluated. Since all-order single-particle functions are used in the present work, important higher-order effects are automatically included in this procedure [22].

The pair correlation can also lead to single-particle effects in higher orders, which can be regarded as a modification of the HF orbitals towards Brueckner orbitals (BO) [22]. Such modifications of the occupied orbitals are evaluated in the present work by means of the first-order pair functions. The new orbitals are then used to re-evaluate the core polarization and the "third-order" diagrams. Using this procedure it is expected that the most important fourth-order effects are included.

The gallium atom is a relatively heavy atom and it is obvious that relativistic effects cannot be neglected in an accurate calculation. No fully relativistic MBPT procedure is yet available and therefore we have applied the following approximate scheme.

The non-relativistic Hartree-Fock, polarization and correlation effects are first evaluated as described above. Then relativistic Hartree-Fock [23] and single-particle [24] programs are used to evaluate the relativistic effects on the HF and the polarization

levels. From these calculations, a “relativistic correction” for the correlation effect is finally estimated and included.

The numerical results obtained in the present work are given in Tables 3–5 and will be further discussed below.

The procedure employed here is quite easy to use, and represents a suitable compromise between accuracy and convenience. The procedure is also designed to include pair-correlation effects to higher orders [25], and it has been applied in this form to hyperfine calculations on some lighter atoms [26]. Such a procedure, however, requires considerably more computer power as well as manpower, and is motivated only when high accuracy is required.

Discussion

From the effective parameters compiled in Table 3 several interesting observations can be made. In the $4p$ state there is a large *negative* spin polarization, while for the higher states this contribution is positive (and decreases with decreasing n). This is evidently due to the large overlap between the $4p$ and $4s$ orbitals, causing a particularly large spin polarization of the $4s$ shell in the ground state. For the same reason there is a particularly large correlation effect in the ground state; this is reduced by one order of magnitude in going from $4p$ to $5p$. In addition, it can be found – as in other similar calculations – that a large fraction ($\sim 80\%$) of the correlation effect, relative to HF, is included in the Brueckner orbitals.

From the comparison between the theoretical and experimental results in Table 4 it is found that the agreement is very good for the ground state but less so for the excited states. Due to the large overlap between the $4p$ and $4s$ orbitals and the large correlation effects in the ground state one would expect a comparatively slow convergence in that state and therefore less accurate results using first-order pair functions. For the excited states, on the other hand, there is reason to believe that such an approximation should be quite adequate. However, the results in Table 4 do not seem to verify these assumptions. The very good agreement obtained for the ground state is probably partly fortuitous. The lack of agreement for the excited states, on the other hand, is more difficult to understand. The relatively small contributions due to the correlation (including the Brueckner-orbital contribution) indicate that the results would not be substantially improved by iterating the pair functions and thereby including pair correlation to higher orders.

Table 3. Theoretical effective hyperfine parameters for ^{69}Ga (in atomic units)

	$\langle r^{-3} \rangle_{01}$	$\langle r^{-3} \rangle_{12}$	$\langle r^{-3} \rangle_{10}$	$\langle r^{-3} \rangle_{02}$
4p				
HF ⁻¹	2.67500	2.67500	0.00000	2.67500
Polarization (HF)	0.20301	0.36505	-3.93925	0.72970
Brueckner orbitals	0.47912	0.47912	0.00000	0.47912
Polarization (BO)	0.02527	0.04087	0.38751	0.07770
Correlation (BO)	-0.08278	-0.09866	2.70912	-0.16447
Total	3.29962	3.46138	-0.84262	3.79706
5p				
HF ⁻¹	0.34740	0.34740	0.00000	0.34740
Polarization (HF)	0.02925	0.04481	0.24890	0.08517
Brueckner orbitals	0.03070	0.03070	0.00000	0.03070
Polarization (BO)	0.01889	0.00114	0.14199	0.00076
Correlation (BO)	-0.00074	-0.00645	0.08346	-0.00200
Total	0.42550	0.41759	0.47435	0.46202
6p				
HF ⁻¹	0.13179	0.13179	0.00000	0.13179
Polarization (HF)	0.01132	0.01688	0.11862	0.03135
Brueckner orbitals	0.00815	0.00815	0.00000	0.00815
Polarization (BO)	0.00050	0.00007	0.04081	-0.00053
Correlation (BO)	0.00004	-0.00262	0.02171	-0.00051
Total	0.15181	0.15428	0.18115	0.17026
7p				
HF ⁻¹	0.06442	0.06442	0.00000	0.06442
Polarization (HF)	0.00558	0.00823	0.06181	0.01513
Brueckner orbitals	0.00334	0.00334	0.00000	0.00334
Polarization (BO)	0.00019	-0.00005	0.01806	-0.00043
Correlation (BO)	0.00031	-0.00111	0.00927	0.00004
Total	0.07384	0.07484	0.08914	0.08251
8p				
HF ⁻¹	0.03626	0.03626	0.00000	0.03626
Polarization (HF)	0.00368	0.00462	0.03578	0.00472
Brueckner orbitals	0.00167	0.00167	0.00000	0.00167
Polarization (BO)	-0.00044	-0.00004	0.00916	-0.00365
Correlation (BO)	0.00022	-0.00099	0.00502	0.00008
Total	0.04139	0.04152	0.04996	0.04617

Similar calculations to those performed here are presently under way for the Al sequence [27]. Here also, higher-order pair correlation effects are included for the ground state as well as for the excited states, and these results may also shed some light on the Ga results presented here. In any case, more advanced calculations on the Ga sequence will not be performed until the Al results have been properly analysed.

Table 4. Hyperfine coupling constants for ^{69}Ga in MHz. (The theoretical B -factors were calculated using the quadrupole moment $Q_{69}=0.178$ barns [17])

	$A_{1/2}$	$A_{3/2}$	$B_{3/2}$
4p			
HF^{-1}	912.3	182.5	44.8
Core polarization	264.8	-156.9	15.2
Correlation	11.8	161.0	3.5
Relativistic effects	162.8	2.0	-2.4
Total	1,351.7	188.6	61.1
Experimental [28]	1,338.994	190.794	62.522
5p			
HF^{-1}	118.5	23.7	5.8
Core polarization	2.0	12.3	1.4
Correlation	3.1	13.4	0.5
Relativistic effects	15.1	-1.2	0.3
Total	138.7	48.2	8.0
Experimental	—	—	—
6p			
HF^{-1}	44.9	9.0	2.2
Core polarization	-0.1	5.7	0.5
Correlation	-0.3	3.3	0.1
Relativistic effects	4.8	0.2	0.1
Total	49.3	18.2	2.9
Experimental [4]	53.3(7)	22.4(2)	3.2(3)
7p			
HF^{-1}	22.0	4.4	1.1
Core polarization	-0.3	3.0	0.2
Correlation	-0.2	1.4	0.1
Relativistic effects	2.3	0.1	0.0
Total	23.8	8.9	1.4
Experimental (this work)	—	11.13(2)	1.52(3)
8p			
HF^{-1}	12.4	2.5	0.6
Core polarization	-0.2	1.7	0.2
Correlation	-0.2	0.8	0.0
Relativistic effects	1.3	0.1	0.0
Total	13.3	5.1	0.8
Experimental (this work)	—	6.35(2)	0.85(1)

Table 5. The effect of grid extrapolation [21] illustrated by the nonrelativistic calculations for the ground state

Points in grid	$A_{1/2}$	$A_{3/2}$	$B_{3/2}$
41	1,195.5	211.5	64.7
51	1,192.7	202.2	64.3
61	1,191.4	197.3	64.1
Extrapolated	1,188.9	186.6	63.5

References

- Jönsson, G., Lundberg, H., Svanberg, S.: Phys. Rev. A **27**, 2930 (1983)
- Jönsson, G., Lundberg, H.: Z. Phys. A - Atoms and Nuclei **313**, 151 (1983)
- Zaki Ewiss, M.A., Snoek, C.: J. Phys. B **16**, L153 (1983)
- Jönsson, G., Levinson, C., Svanberg, S., Wahlström, C.-G.: Phys. Lett. **93A**, 121 (1983)
- Jiang Zhan-Kui, Lundberg, H., Svanberg, S.: Phys. Lett. **92A**, 27 (1982)
- Jiang Zhan-Kui, Lundberg, H., Svanberg, S.: Z. Phys. A - Atoms and Nuclei **306**, 7 (1982)
- Jönsson, G., Kröll, S., Lundberg, H., Svanberg, S.: Z. Phys. A - Atoms and Nuclei **316**, 259 (1984)
- Neijzen, J.H.M., Dönszelmann, A.: Physica **98C**, 143 (1979)
- Neijzen, J.H.M., Dönszelmann, A.: Physica **114C**, 395 (1982)
- Lindgren, I., Morrison, I.: Atomic many-body theory. In: Springer Series in Chemical Physics. Vol. 13. Berlin, Heidelberg, New York: Springer 1982
- Belfrage, Ch., Hörbäck, S., Levinson, C., Lindgren, I., Lundberg, H., Svanberg, S.: Z. Phys. A - Atoms and Nuclei **316**, 15 (1984)
- Young, W.A., Mirza, M.Y., Duley, W.W.: Opt. Commun. **34**, 353 (1980)
- Farley, J., Wing, W.H.: Phys. Rev. A **23**, 2397 (1981)
- Gallagher, T.F., Cooke, W.E.: Phys. Rev. Lett. **42**, 835 (1979)
- Dodd, J.N., Series, G.W.: Progress in Atomic Spectroscopy. Part A. Hanle, W., Kleinpoppen, H. (eds.). New York: Plenum Press 1979
- Ramirez, R.W.: The FFT: Fundamentals and Concepts. Tektronix Inc 1975
- CRC Handbook of Chemistry and Physics. 61st Edn. Boca Raton: CRC Press Inc 1981
- See, for instance, Lindgren, I., Rosén, A.: Case Stud. At. Phys. **4**, 93 (1974)
- Sternheimer, R.M.: Phys. Rev. **80**, 102 (1950)
- Garpman, S., Lindgren, I., Lindgren, J., Morrison, J.: Z. Phys. A - Atoms and Nuclei **276**, 167 (1976)
- Morrison, J.: J. Phys. B **6**, 2205 (1973)
- Garpman, S., Lindgren, I., Lindgren, J., Morrison, J.: Phys. Rev. A **11**, 758 (1975)
- Lindgren, I., Lindgren, J., Mårtensson, A.-M.: Z. Phys. A - Atoms and Nuclei **279**, 113 (1976)
- Rosén, A., Lindgren, I.: Phys. Rev. **176**, 114 (1968)
- Heully, J.-L., Mårtensson-Pendrill, A.-M.: Phys. Scr. **27**, 291 (1983); Phys. Rev. A **27**, 3332 (1983)
- Mårtensson, A.-M.: J. Phys. B **12**, 3995 (1979)
- Lindgren, I.: Phys. Rev. A **31**, 1273 (1985)
- Salomonsson, S.: Z. Phys. A - Atoms and Nuclei **316**, 135 (1984)
- Mårtensson-Pendrill, A.-M., Salomonsson, S.: Phys. Rev. A **30**, 712 (1984)
- Hörbäck, S., Lindgren, I.: (to be published)
- Daly, R.T., Holloway, J.H.: Phys. Rev. **96**, 539 (1954)
- Lurio, A., Prodell, A.G.: Phys. Rev. **101**, 79 (1956)

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PAPER VI

Hyperfine Structure Studies in 2D and 4P States of ^{27}Al , $^{69,71}\text{Ga}$ and ^{115}In

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The hyperfine structure of the lowest ns^2nd 2D states in ^{27}Al , $^{69,71}\text{Ga}$ and ^{115}In and of the $5s5p^2$ 4P states of ^{115}In was measured using high-resolution laser spectroscopy on atomic beams. Intra-cavity frequency doubling was employed. The results were analysed using the Multi-Configuration Hartree-Fock method.

PACS: 31.30G

1. Introduction

The hyperfine structures (hfs) and radiative lifetimes of the 2D sequences in the group III A elements have attracted a considerable interest. The lifetimes have been studied extensively both experimentally and theoretically [1–3] and have been found strongly affected by configuration interaction with the sp^2 configurations. Hfs has been measured to a much lesser extent. Zimmermann and coworkers determined the hfs in the low 2D states in Al and In using the level-crossing technique some ten years ago [4, 5]. The results deviated from what can be expected from a central-field model.

In the present paper we report on investigations of the lowest $^2D_{3/2,5/2}$ states of ^{27}Al , $^{69,71}\text{Ga}$ and ^{115}In and in the $5s5p^2$ 4P states of In. The experiments were performed using a cw UV laser beam acting on a collimated atomic beam. Theoretical calculations were performed for all the studied states using the Multi-Configuration Hartree-Fock method.

2. Measurements

In the experiments laser excitation of an atomic beam was employed. The atomic beam was produced in a vacuum system using a resistively heated oven. The wavelengths of the transitions from the ground states to the lowest 2D states in Al, Ga and In are in the region 280–330 nm. Light on these wavelengths was

obtained by intra-cavity frequency doubling in a ring dye-laser operated in yellow and red (CR-7500). A LiIO_3 or a KDP crystal and a UV beam-splitter were placed in the dye-laser cavity and the standard output coupler was replaced by a high reflector. Typically a single-mode UV-power of 0.5 mW was obtained.

The experimental set-up is shown in Fig. 1. The visible light leaking through the high reflector was used to monitor the laser performance and frequency. The UV beam irradiated the collimated atomic beam at right angle and the fluorescence was detected by a photo-multiplier. In the measurements the rough wavelengths were set using table values and the wavelength meter. The laser wavelength was then scanned over the hfs components and the fringes from the Fabry-Pérot interferometer were recorded simultaneously. A curve for the $5s^25p^2P_{3/2} - 5s5p^2^4P_{3/2}$ transition in ^{115}In is shown in Fig. 2. For each state a number of recordings were made and the evaluation was performed using the known splitting of the ground state as calibration. In some states the hfs components were incompletely resolved and then a fit procedure was employed. For the two Ga isotopes the ratio between the nuclear moments was used in the evaluation. The isotope shifts $\nu_{71} - \nu_{69}$ in the transitions $4s^24p^2P_{1/2} - 4s^24d^2D_{3/2}$ and $4s^24p^2P_{3/2} - 4s^24d^2D_{5/2}$ were found to be 123(20) MHz and 100(20) MHz, respectively. The results for the magnetic-dipole- and electric-quadrupole coupling constants A and B are given in Tables 1 and 2. The com-

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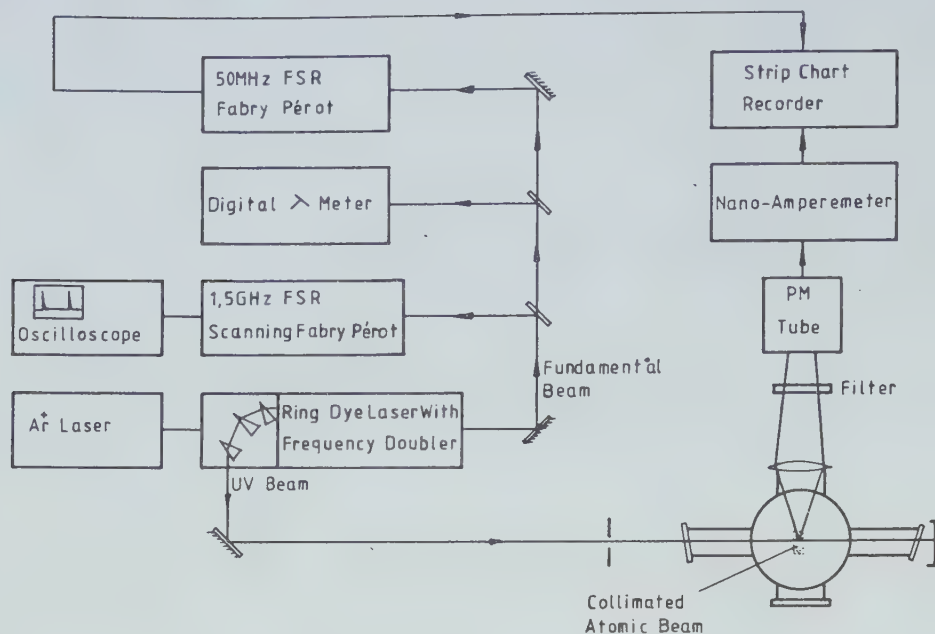


Fig. 1. Experimental set-up

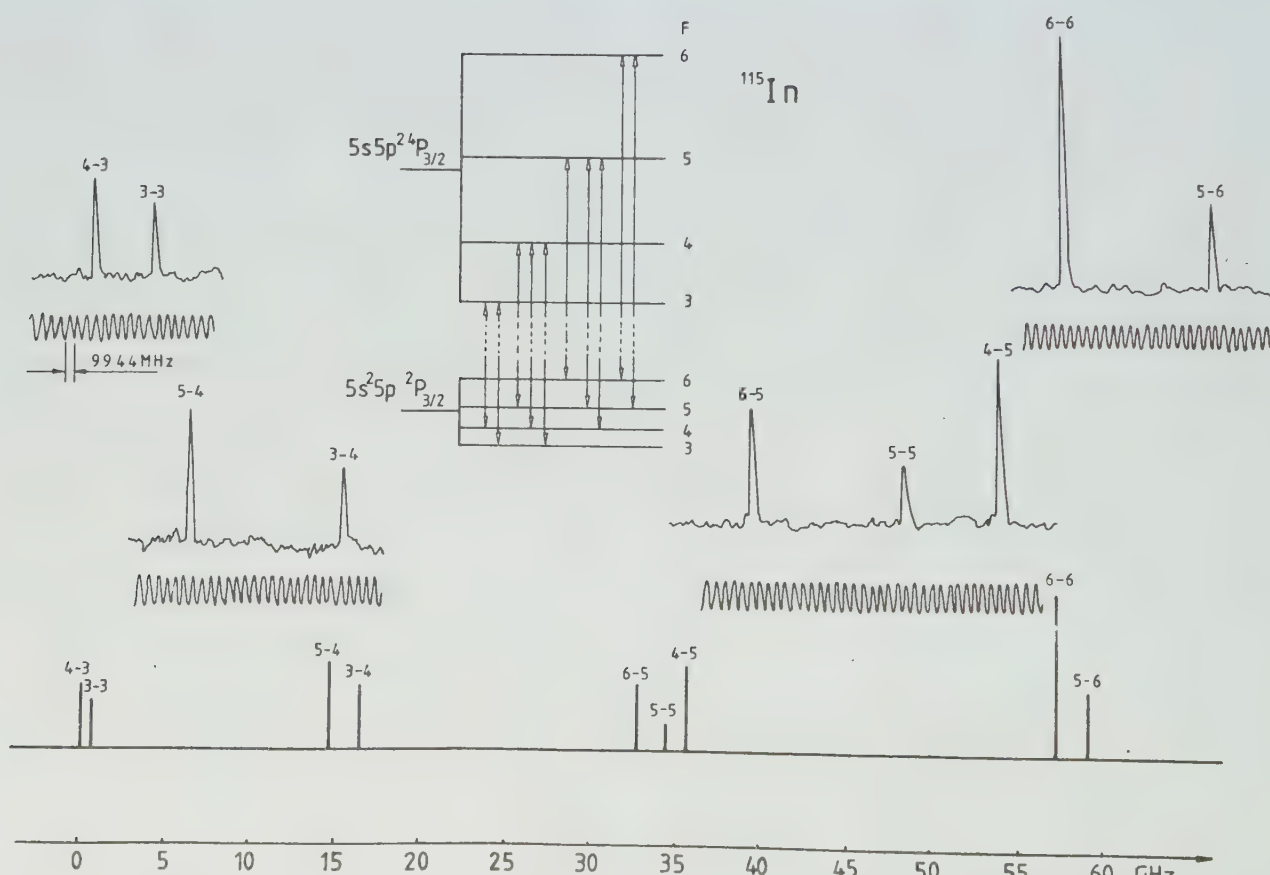
Fig. 2. An experimental recording of the $5s^2 5p^2 \text{ } ^2\text{P}_{3/2} - 5s 5p^2 \text{ } ^4\text{P}_{3/2}$ transition in ^{115}In . A hyperfine transition diagram is included

Table 1. Theoretical A-factors and experimental A- and B-factors for the 2D states. The first column gives the values from single configuration Hartree-Fock calculations. Column 7 gives the contributions from the sp^2 perturber to the total theoretical A-factors in column 8

	A (MHz) Hartree- Fock	C_1^2	C_2^2	C_3^2	$C_1^2 + C_2^2 + C_3^2$	$A(sp^2)$	$C_3^2 A(sp^2)$	$A(s^2d + p^2d + sp^2)$	Experimental	
									A(MHz)	B(MHz)
^{27}Al $^2D_{3/2}$	1.0					-360.9	-78.3	-75.7	-99(4)	15 (15)
^{27}Al $^2D_{5/2}$	0.4	0.7269	0.0420	0.2171	0.9860	723.9	157.2	158.3	185(5)	-20 (40) ^a
^{69}Ga $^2D_{3/2}$	2.4					-1,186.6	-57.1	-51.6	-38(3)	9 (7)
^{69}Ga $^2D_{5/2}$	1.0	0.9044	0.0414	0.0481	0.9939	2,017.1	97.0	99.4	76(4)	14 (10)
^{115}In $^2D_{3/2}$	2.6					-1,413.8	-96.6	-86.8	-62(4)	40 (40)
^{115}In $^2D_{5/2}$	1.0	0.8858	0.0448	0.0683	0.9989	2,496.7	170.5	175.0	152(2)	40 (50)

^a According to the non-relativistic theory of effective operators [15], applied to electric-quadrupole interaction, the B-factors of $^2D_{3/2}$ and $^2D_{5/2}$ have the same sign and a ratio of 10/7. A positive sign is within the experimental error bars

Table 2. Theoretical and experimental values for the A and B factors in the $5s5p^2\ ^4P$ states of ^{115}In

	Hartree-Fock				Experimental	
	non-relativistic		relativistic		A(MHz)	B(MHz)
	A(MHz)	B(MHz)	A(MHz)	B(MHz)		
$^4P_{5/2}$	2,242	-574	3,318	-644	3,689 (20)	-638 (50)
$^4P_{3/2}$	2,434	459	3,675	458	3,998 (20)	427 (50)
$^4P_{1/2}$	5,128		8,040		9,193 (50)	

paratively large errors for the B factors are due to the small coefficients in the equations in A and B giving the splittings. A good agreement with the values of Zimmermann et al. (Al and absolute values for In 2D) exists.

3. Analysis

In a central-field model the A factors for the $ns^2nd\ ^2D$ states have the ratio $A(^2D_{5/2})/A(^2D_{3/2}) = 3/7$ and they should all be positive since the corresponding nuclear magnetic moments are positive. The experimental A factors, however, are at least one, and often two, orders of magnitude larger than that which one obtains using the restricted Hartree-Fock model. Further, the experimental A factors for the $^2D_{3/2}$ states are negative for all three elements.

A theoretical study of these 2D states, including core polarization, pair correlations and relativistic effects using many body perturbation theory (MBPT) is in progress [6]. Our aim in this section is not to give a complete analysis of the investigated states, but merely to give an explanation of the large absolute values and the inverted structure of the $^2D_{3/2}$ states.

As already pointed out by Falkenburg and Zimmermann for aluminium [4], the admixture of the perturbing $nsnp^2\ ^2D$ state plays a dominant role for

these A factors. Configurations with unpaired s-electrons always give large contributions to the magnetic hyperfine structure because of the Fermi contact interaction. It is therefore necessary to know how large these admixtures are in the different elements investigated when we want to calculate the A factors. We have performed nonrelativistic calculations of the wavefunctions with the Multi-Configuration Hartree-Fock method (MCHF) [7] using the computer codes of Froese Fischer [8].

For all three elements the $nsnp^2$ configuration gives the second largest component in the MCHF wavefunctions. When performing the calculations of the wavefunction it is not sufficient to include the most important configurations in order to minimize the total energy. The correct energy of the $nsnp^2$ perturber relative to the $ns^2nd\ ^2D$ state is essential to get correct mixing coefficients. Here we were guided by energy values from quantum defect analyses [9-11] and photo-absorption measurements [12, 13].

In Table 1 the single-configuration Hartree-Fock and MCHF values for the A factors together with the experimental A and B factors are presented. The Table also gives the square of the mixing coefficients for the three largest components in the MCHF wavefunction

$$\psi_{tot} = C_1 (s^2d)^2D + C_2 (p^2(^1S)d)^2D + C_3 (sp^2)^2D + \dots$$

The total number of configurations included in the MCHF wavefunctions was 12 in Al, 12 in Ga and 8 in In. As indicated in Table 1, the three largest components account for nearly 100% of the total wavefunction for all three elements.

In Table 1 the contributions to the A factors from sp^2 are listed separately in columns 6 and 7. This clearly demonstrates that the admixture of sp^2 gives rise to the large absolute values of the A factors as well as the inverted structures for the $J=3/2$ states.

The hyperfine interaction, being represented by one-body operators [14], can only connect configurations differing by, at most, one electron. In a perturbation expansion the effect of sp^2 will therefore be present first in third-order (second in electrostatic and first in hyperfine interactions). Different types of core polarization, which would be represented already in second order in a perturbation expansion, are neglected in this work since we are treating the shells in the electron core as spherically symmetric. Preliminary results from the MBPT calculation [6] show that the effect of core polarization cancels part of the contribution from sp^2 . It gives positive contributions to the A factors of the $J=3/2$ states and negative contributions to the A factors of the $J=5/2$ states. This "cancellation effect" is largest for the $J=3/2$ states, but not larger than about 5% in Al and 20% in In. Relativistic effects can not be expected to be negligible for Ga and In, but are not included in this study of the 2D states.

An MCHF calculation for the experimentally investigated $5s5p^2\ ^4P$ state in In showed that this state is practically pure (99% $5s5p^2$). In Table 2 we therefore present, together with the experimental results, theoretical A and B factors for this state from single-configuration Hartree-Fock calculations. The calculations were performed non-relativistically as well as

relativistically and the results of both methods are presented.

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References

1. Weiss, A.W.: Phys. Rev. **A9**, 1525 (1974)
2. Carlsson, J., Lundberg, H., Peng, W.X., Persson, A., Wahlström, C.-G., Brage, T., Froese Fischer, C.: Z. Phys. **A-Atomic Nuclei** **331**, 111 (1986)
3. Zaki Ewiss, M.A., Snoek, C., Dönszelmann, A.: Astron. Astrophys. **121**, 327 (1983)
4. Falkenburg, B., Zimmermann, P.: Z. Naturforsch. **34a**, 1249 (1979)
5. Brieger, M., Bucka, H., Reichelt, A., Zimmermann, P.: Z. Naturforsch. **24a**, 903 (1969)
6. Salomonsen, J., Wahlström, C.-G.: (to be published)
7. Froese Fischer, C.: The Hartree-Fock method for atoms. New York: Wiley 1977
8. Froese Fischer, C.: US Department of Energy report No. DOE/ER/10618-11 (1983)
9. Lin, C.D.: Astrophys. J. **187**, 385 (1974)
10. Neijssen, J.M.H., Dönszelmann, A.: Physica **114C**, 399 (1982)
11. Vlieger, G.J.N.E. de, Wijnen, H., Dönszelmann, A.: Physica **121C**, 241 (1983)
12. Kozlov, M.G., Startsev, G.P.: Opt. Spectrosc. **24**, 3 (1968)
13. Connerade, J.P., Baig, M.A.: J. Phys. **B14**, 29 (1981)
14. Lindgren, I., Rosén, A.: Case Stud. At. Phys. **4**, 93 and 197 (1974)
15. Lindgren, I.: Rep. Prog. Phys. **47**, 345 (1984)

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PAPER VII

Hyperfine-dependent lifetimes induced by singlet-triplet mixing

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The effect of hyperfine-induced singlet-triplet mixing on radiative lifetimes has been studied in neutral strontium. Different lifetimes are, for the first time, observed for different hyperfine components in laser-spectroscopy measurements combining high spectral and temporal resolution. The experimental results are found to be in good agreement with theoretical calculations.

Natural radiative lifetime measurements can, under certain circumstances, serve the purpose of investigating the composition of atomic wave functions. In particular, the lifetime values obtained for sequences of normally long-lived Rydberg states sensitively reflect the admixture of short-lived doubly excited states. Particularly spectacular effects are obtained for the $6sns\ ^1S_0$ and $6snd\ ^1D_2$ sequences of Ba.¹⁻⁴ Natural radiative lifetimes do not normally show any dependence on the F quantum number within a state, since the lifetime is an electronic quantity and has nothing to do with the nuclear properties. However, there can be such a dependence due to hyperfine-induced mixing between levels with different radiative lifetimes. In the present paper such effects are demonstrated for the first time.

During recent years hyperfine-induced singlet-triplet mixing has been studied, particularly for He (Ref. 5) and in sequences of the alkaline earths.⁶⁻⁸ In these studies the influence of the hyperfine structure (hfs) has been used to probe the interaction. There have also been reports on transition probabilities affected by this kind of hyperfine-induced mixing in Hg and more recently in OVII and Fe VIII.⁹ Beigang *et al.*¹⁰ report a strong localized singlet-triplet mixing between the series $5snd\ ^1D_2$ and $5snd\ ^3D_3$ for $n = 19$ in ^{87}Sr . These are the states investigated in the present work regarding F -dependent lifetimes.

The difference in energy ΔE between these two states is comparable to the Fermi contact term a_{5s} of the inner s electron, leading to the local mixing. The effect can only exist in the ^{87}Sr isotope ($I = \frac{9}{2}$, natural abundance 7.02%), since it is the only stable one having a nonzero nuclear magnetic moment. On the other hand, measurements on the even isotopes, e.g., ^{88}Sr (natural abundance 82.56%), give the unperturbed lifetimes for the singlet and the triplet states. We describe lifetime measurements on individual hfs components of ^{87}Sr and on the unperturbed states of ^{88}Sr . In order to measure lifetimes of individual hfs components, one must have high-energy resolution as well as high temporal resolution. Therefore, a delayed coincidence method employing a pulse-modulated cw single-mode dye laser was used. This scheme, referred to as PUMOLS (pulse modulated laser spectroscopy), has been applied previously for radiative lifetime measurements on Rydberg sequences in Sr and Ba.^{1,2,11,12}

The PUMOLS technique has been described in detail

earlier,¹³ but a brief description of the method used is presented here. In PUMOLS experiments cw laser light is used to excite free atoms in an atomic beam. The light is externally pulse-modulated at high repetition rates. Suitable pulse lengths and light-off intervals are set depending on the individual lifetimes, i.e., approximately 3τ and 10τ , respectively. The fluorescence photons are detected in a photomultiplier tube (PMT). It is essential that each laser pulse gives rise to, at the most, one fluorescence photon at the detector. These photons give the stop signals to a time-to-amplitude converter (TAC) started with trigger pulses directly from the pulse modulator. Necessary precautions, as discussed in Ref. 13, regarding, e.g., pile up, multiple scattering, and distortion by Zeeman quantum beats, must be taken. A multichannel analyzer (MCA) is used for sampling the decay photons and the completed curves are stored in a computer for later evaluation.

In neutral strontium, two-step excitation from the $5s^2\ ^1S_0$ ground state to the $5s\ 19d\ ^1D_2$ Rydberg state, via the $5s\ 5p\ ^1P_1$ intermediate state was employed, as illustrated in Fig. 1. The actual experimental setup used is shown in Fig. 2. For the first step, at 460.7 nm, a multimode dye laser (Coherent Radiation CR 599) running on Coumarin 470 was used. An uv krypton-ion laser (CR 3000 K) was utilized as a pump. To achieve "white" excitation of the intermediate state, the piezo-mounted folding mirror of the dye laser was scanned rapidly with a voltage ramp to smear out the mode structure of the laser. A Stilbene 3 single-mode ring dye laser (CR 699-21) pumped by an argon-ion laser (Spectra Physics SP-171-18) was used for the second step. The light from the ring laser was pulse-modulated externally by an acousto-optic modulator (SORO-MAR-50). The linewidth of the single-mode laser (normally 1 MHz) was only slightly affected by Fourier broadening due to the pulsing, since the pulse length was 1 μs or longer. The strontium atomic beam was produced in a resistively heated oven, inside a vacuum chamber. The excitation was performed at right angles to the atomic beam, which was collimated with apertures to a ratio of about 1:20 for reduction of the Doppler width. The optical detection system, orthogonal to both the atomic and laser beams, consisted of appropriate color and interference filters, together with a Peltier-cooled PMT (EMI 9558 QB).

Since the $19d\ ^3D_3$ state for the even isotopes cannot be excited from the $5s\ 5p\ ^1P_1$ level, the metastable state

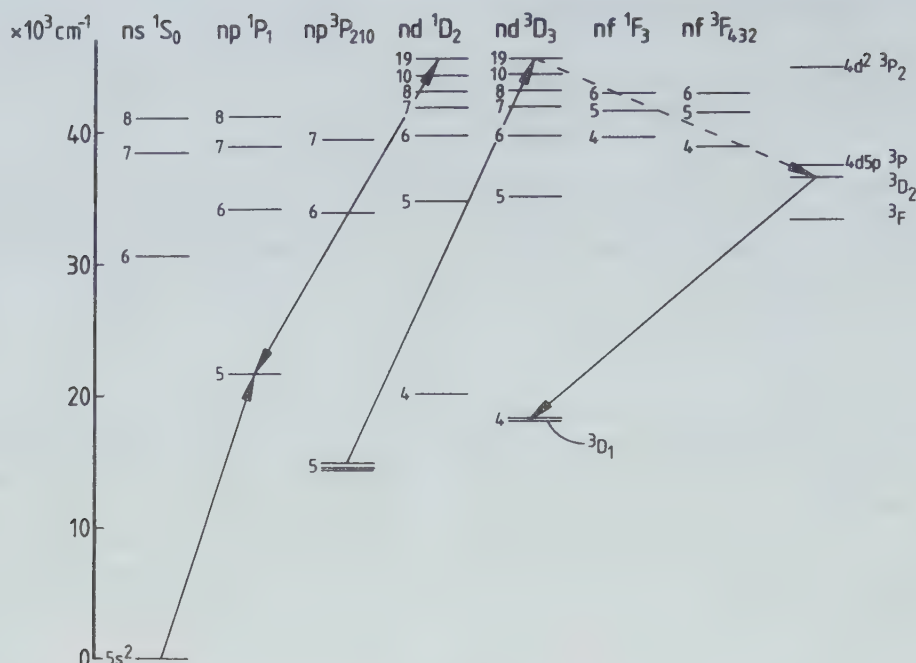


FIG. 1. Schematic energy-level diagram for neutral strontium. The transitions used for excitation and detection are indicated.

$5s5p^3P_2$ had to be used. This called for a pulsed laser system as the wavelength was in the uv region (326.4 nm). The metastable population was achieved by applying a discharge in the atomic beam about 1 cm above the oven, and letting the released electrons collide with the atoms. A Nd-YAG (yttrium aluminum garnet) pumped dye laser (Quanta-Ray DCR-2 and PDL-1) and a Raman shifter (Quanta-Ray RS-1) were then used to excite the atoms to the triplet state. The decay was recorded with a transient recorder (Biomation 8100) and an external mass memory in which the transients were added. However, the route of decay was not as expected. It was found that the 3D_3 state mainly decayed through transitions involving both

valence electrons. There was no distinguishable fluorescence at the laser wavelength, but a strong signal was found at the wavelength of the $4d5p^3D_2-5s4d^3D_1$ line. This decay route is indicated in Fig. 1. The lifetime deduced from this cascade can be trusted since the intermediate doubly excited state has a much shorter lifetime than the $19d^3D_3$ state.

The hyperfine structures of the $18-20d^1D_2$ states were recorded by scanning the single-mode laser, and they were found to be in agreement with those obtained in Ref. 10. Only in the $19d$ scan did extra peaks appear. The peaks belong to the $19d^3D_3$ state and have F quantum numbers from $\frac{5}{2}$ to $\frac{13}{2}$. The triplet components with $F = \frac{3}{2}$ and $\frac{15}{2}$ do not mix into the singlet and consequently will not be seen in a scan of the $19d^1D_2$ state. The lifetimes were then measured for different F components. No F dependence was found for $18d$ and $20d$, while for the $19d$ state pronounced differences were observed. Possible systematic errors were minimized by performing measurements on the hfs components with equal detected signal strengths, achieved through laser-beam intensity regulation, for constant atomic density. Further, the even-isotope singlet signal and the ^{87}Sr hfs component signals ($^1D_2, ^3D_3$) were measured alternately.

Due to low signal strength the atomic beam could not be sufficiently collimated to reduce the Doppler broadening enough to resolve the $F = \frac{11}{2}$ and $\frac{13}{2}$ components of the singlet state. Therefore, one value is given for these components and it should be interpreted as a weighted mean of the two individual values.

In Fig. 3 two experimental curves can be seen which show the difference in lifetime for the unresolved $F = \frac{11}{2}$ and $\frac{13}{2}$ peak, and the $F = \frac{9}{2}$ peak for ^{87}Sr . All components belong to the $19d^1D_2$ state. The measured lifetime values for selected hyperfine components and the two ^{88}Sr values are compiled in Table I.

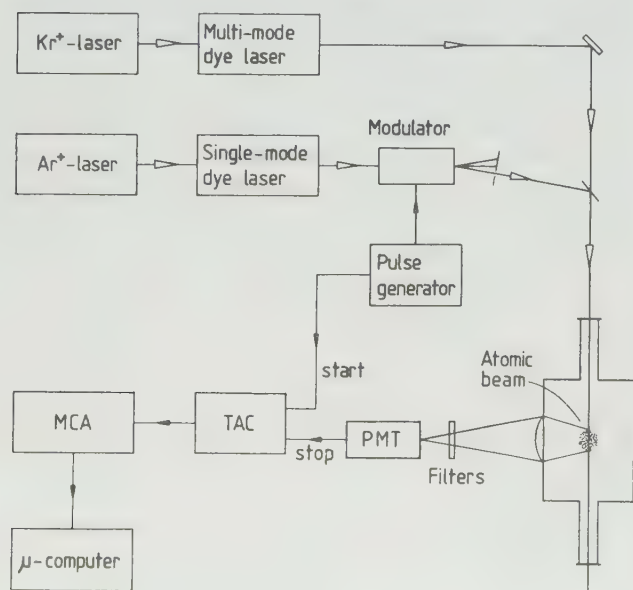


FIG. 2. Experimental setup for the PUMOLS measurements.

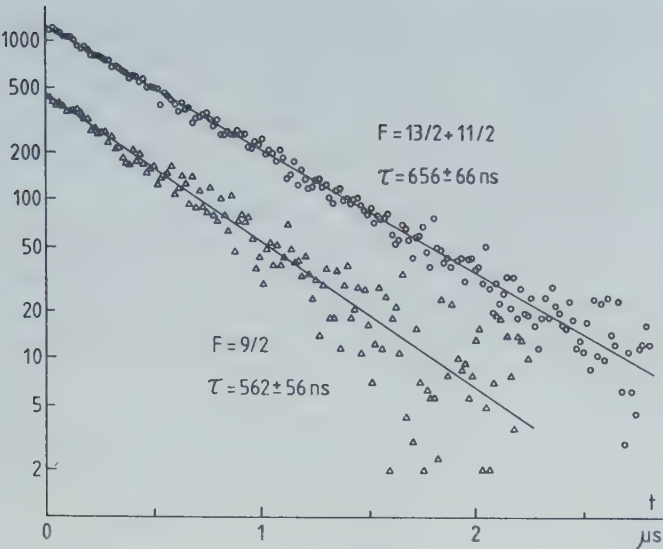


FIG. 3. Experimental decay curves for two hyperfine peaks, belonging to the $19d\ ^1D_2$ state, shown on a $\log_{10}$ -linear plot with the best fit (drawn line). Background counts have been subtracted.

The wave functions Ψ for the odd-isotope hfs component with a specific F number can be written approximately as linear combinations of the unperturbed wave functions $\bar{\Psi}$ for the even isotopes

$$\begin{aligned}\Psi(^1D_2'', F) &= a_F \bar{\Psi}(^1D_2) + b_F \bar{\Psi}(^3D_3), \\ \Psi(^3D_3'', F) &= -b_F \bar{\Psi}(^1D_2) + a_F \bar{\Psi}(^3D_3).\end{aligned}$$

When calculating transition probabilities from these mixed states to a given lower state $\bar{\Psi}_0$, one obtains cross terms for constructive and destructive interference. When

TABLE I. Observed lifetimes.

Isotope	State	hfs level	τ . (ns)
^{88}Sr	1D_2		766 ± 77
	3D_2		395 ± 79
^{87}Sr	" 1D_2 "	$(F = \frac{13}{2}) + (F = \frac{11}{2})$	656 ± 66
		$F = \frac{9}{2}$	562 ± 56
	" 3D_2 "	$F = \frac{5}{2}$	652 ± 65
		$F = \frac{7}{2}$	583 ± 58

lifetimes are calculated, however, summation over the F components of the lower level is carried out and the interference terms cancel. For the radiative decay rates Γ one obtains

$$\begin{aligned}\Gamma(^1D_2'', F) &= a_F^2 \bar{\Gamma}(^1D_2) + b_F^2 \bar{\Gamma}(^3D_3), \\ \Gamma(^3D_3'', F) &= b_F^2 \bar{\Gamma}(^1D_2) + a_F^2 \bar{\Gamma}(^3D_3).\end{aligned}$$

Here $\bar{\Gamma}$ denotes the decay rate of the corresponding pure states in the even isotopes. If the radiative lifetimes of the 1D_2 and 3D_3 states are different in the even isotopes, as was found in ^{88}Sr , one will obtain, for the mixed states, decay rates that depend on the hyperfine-induced mixing coefficients a_F and b_F .

To obtain the mixing coefficients the Fermi contact term $W = a_{5s} \mathbf{I} \cdot \mathbf{s}$ was added to the total Hamiltonian $H = H_0 + W$. The energy matrix, which breaks up into 2×2 submatrices, one for each F value (except for $F = \frac{3}{2}$ and $\frac{15}{2}$, which do not mix, since there are no such states for 1D_2), was then diagonalized. In a purely LS -coupled 1D_2 state there will be no hyperfine splitting.¹⁴ For Sr,

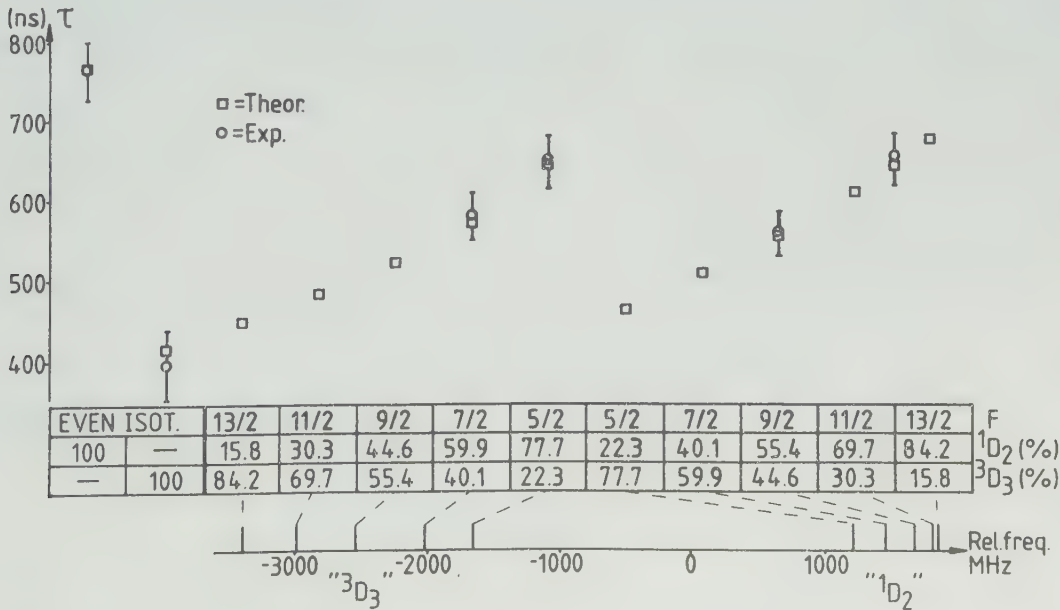


FIG. 4. Comparison between the theoretical and experimental lifetime results. The eigenvector composition is shown at the bottom of the figure, together with a schematic representation of the relative positions for the hyperfine components. The energy structure is taken from Ref. 9.

however, intermediate coupling exists. Before setting up the energy matrix the wave function for the 1D_2 state therefore has to be expanded in wave functions for purely *LS*-coupled states; $^3D_2^o$ and $^1D_2^o$.¹⁴

$$\Psi(^1D_2) = \alpha' \Psi(^3D_2^o) + \beta' \Psi(^1D_2^o) .$$

Values for α' and β' are found in the literature.^{10,15}

The mixing coefficients and energy eigenvalues depend critically on the separation between the centers of gravity of the unperturbed 3D_3 and 1D_2 levels. We used the value $\Delta E = 1.78$ GHz found by Beigang *et al.*¹⁰ when studying the energy structures.

Figure 4 shows the theoretical and experimental lifetime results. As can be seen, good agreement between the values is found. The squares of the calculated hyperfine-

induced mixing coefficients a_F and b_F are also indicated in the figure. From these numbers it can be deduced that the designation of the $F = \frac{5}{2}$ and $\frac{7}{2}$ states, labeled " 1D_2 " and " 3D_3 " in the figure, should really be interchanged if the states are named according to dominant eigenvector components.

In conclusion, we have for the first time experimentally shown and theoretically interpreted how *F*-dependent lifetime values can occur as a result of strong hyperfine-induced level mixing. The observations give further insight into hyperfine-induced perturbations, that have so far only been studied using hfs level shifts.

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¹M. Aymar, P. Grafström, C. Levinson, H. Lundberg, and S. Svanberg, *J. Phys. B* **15**, 877 (1982).

²K. Bhatia, P. Grafström, C. Levinson, H. Lundberg, L. Nilsson, and S. Svanberg, *Z. Phys. A* **303**, 1 (1981).

³T. F. Gallagher, W. Sandner, and K. A. Safinya, *Phys. Rev. A* **23**, 2969 (1981).

⁴M. Aymar, R.-J. Champeau, C. Delsart, and J. C. Keller, *J. Phys. B* **14**, 4489 (1981).

⁵P. F. Liao, R. R. Freeman, R. Panock, and L. M. Humphrey, *Opt. Commun.* **34**, 195 (1980).

⁶H. Rinneberg, *Z. Phys. A* **302**, 363 (1981).

⁷R. Beigang, E. Matthias, and A. Timmermann, *Phys. Rev. Lett.* **47**, 326 (1981).

⁸R. Beigang and A. Timmermann, *Phys. Rev. A* **25**, 1496 (1982).

⁹L. Engström, C. Jupén, B. Denne, S. Hultdt, Weng Tai Meng,

P. Kaijser, U. Litzén, and I. Martinson, *J. Phys. B* **13**, L143 (1980) and references therein; L. Engström, C. Jupén, B. Denne, S. Hultdt, Weng Tai Meng, P. Kaijser, J. O. Ekberg, U. Litzén, and I. Martinson, *Phys. Scr.* **22**, 570 (1981).

¹⁰R. Beigang, D. Schmidt, and A. Timmermann, *J. Phys. B* **15**, L201 (1982).

¹¹P. Grafström, Jiang Zhan-Kui, G. Jönsson, C. Levinson, H. Lundberg, and S. Svanberg, *Phys. Rev. A* **27**, 947 (1983).

¹²G. Jönsson, C. Levinson, A. Persson, and C.-G. Wahlström, *Z. Phys. A* **316**, 255 (1984).

¹³M. Gustavsson, H. Lundberg, L. Nilsson, and S. Svanberg, *J. Opt. Soc. Am.* **69**, 984 (1979).

¹⁴A. Lurio, M. Mandel, and R. Novick, *Phys. Rev.* **126**, 1758 (1962).

¹⁵P. Esherick, *Phys. Rev. A* **15**, 1920 (1977).

PAPER VIII

Natural Radiative Lifetimes in the 1P_1 and 1F_3 Sequences of Sr I

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We have measured radiative lifetimes in the $5sn p\ ^1P_1$ ($n=5-29$) and $5sn f\ ^1F_3$ ($n=4-11$) Rydberg series in neutral strontium. The measurements were performed with single-step laser excitation starting from the ground state or from a metastable state populated by collisions. The decay photons were detected using delayed coincidence technique or a transient recorder. The presence of configuration interaction in the $5sn p\ ^1P_1$ series can be observed around $n=8$. The perturbation in the $5sn f\ ^1F_3$ series is not reflected in the behaviour of the lifetime values.

Introduction

In the alkaline-earth atoms, lifetime measurements have successfully been used to probe effects of configuration interaction. Lifetime values in a Rydberg series are expected to scale with a power close to three of the effective principal quantum number. The presence of a short-lived perturbing state can cause large deviations from this rule [1]. If a series has several perturbers or if the perturbation is spread out over a number of states the effect may be less drastic. Previous lifetime measurements show, that the $5snd\ ^1D_2$ series in Sr I is perturbed in a complex way [2, 3].

Both the 1P_1 and 1F_3 series can be reached with single-step laser excitation starting from the metastable $5s4d\ ^1D_2$ state. In an atomic beam, collisions in a discharge populate all the metastable states. CW laser light from 403 nm to 707 nm was produced using different dyes. With the PUMOLS (Pulse MOdulated Laser Spectroscopy) technique we measured lifetimes in the $5sn p\ ^1P_1$ ($n=7-12$) and $5sn f\ ^1F_3$ ($n=4-11$) series [1]. The 1P_1 series can also be reached from the $5s^2\ ^1S_0$ ground state in a single step if short wavelengths can be generated. With an excimer laser system we measured the 1P_1 series up to $n=29$, corresponding to wavelengths down to 218 nm. Photons released in the decay were detected with a photomultiplier tube and a transient recorder. Some lifetime values for the lower lying states in the 1F_3 series have earlier been measured with laser

spectroscopy techniques [2, 4]. These results agree with ours. In the 1P_1 sequence four states have previously been measured [5]. Our results consistently determined with both the mentioned techniques show large deviations from the published values for $n=6-8$.

Experimental Techniques

The experimental arrangements used in this work are similar to the ones described in [1, 6]. A resistively heated oven produced an atomic beam and through collisions in a discharge the metastable $5s4d\ ^1D_2$ and $^3D_{3,2,1}$ states could be populated.

In the PUMOLS experiments an Argon- or Krypton ion laser (Spectra Physics SP 171-18 or Coherent Radiation CR 3000 K) was used to pump a dye laser (Coherent Radiation CR 599 or CR 699). To get an effective pumping of the various laser dyes either UV, violet, green or red ion laser lines were employed. With the following dyes, laser light with wavelengths from 403 nm to 707 nm was produced: Stilbene 1, Stilbene 3, Coumarin 1, Coumarin 30, Rhodamine 110 and Oxazine 1. The dye laser was not always used with a single cavity mode. If multi-mode operation was chosen, the folding mirror was piezo-electrically vibrated to get an effectively white excitation of the studied state. The dye-laser light

was modulated by an acousto-optic modulator (SORO-MAR-50). It should be noticed, that the crystal in the modulator absorbs light with wavelengths shorter than 400 nm. The modulator was controlled by a pulse generator (HP-8013 B), which also provided a start pulse for the time-to-amplitude converter (TAC). The pulse length and pulse repetition rate was individually set for each studied state. The fluorescence photons passed through interference filters and were detected by a Peltier-cooled photomultiplier tube (EMI 9558 QB). The first detected photon caused a stop signal to the TAC. The decay curves were sampled in a multichannel analyzer (Tracor Northern TN 1710) and the lifetime values were calculated on a mini-computer (PDP-11V03).

In the pulsed laser experiments an excimer laser (Lambda Physik EMG 102) operating with XeCl pumped a dye laser (Lambda Physik FL 2002) using Coumarin 120, Coumarin 47, Coumarin 30 or Rhodamine 6G dye. The dye laser light was frequency doubled with a KD*P- or a KPB-crystal. In this way states corresponding to wavelengths between 218 nm and 293 nm could be reached. Decay photons passed through interference filters and were detected by a fast photomultiplier tube (EMI 9816 QB). The decay signal was captured by a transient digitizer (Biomation 8100). The transients were added in a memory and transferred to the mini-computer for calculations.

Measurements and Results

Figure 1 shows the excitation scheme used in the experiment. The $5snf\ ^1F_3$ sequence was excited from

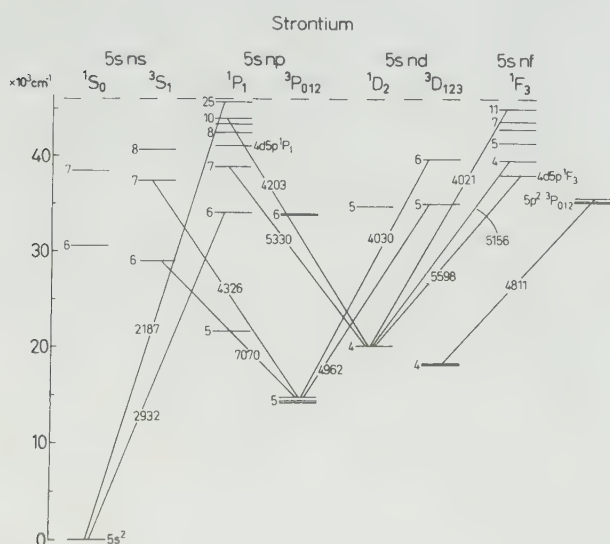


Fig. 1. Excitation scheme in the Sr I spectrum

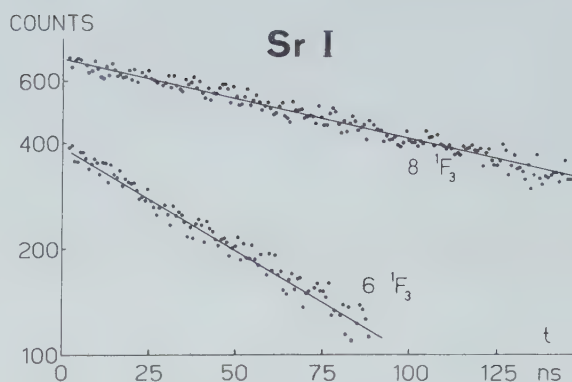


Fig. 2. Two experimental PUMOLS curves recorded with the dye laser running multi mode, drawn on a logarithmic scale. Each curve has a sampling time of about 2 min

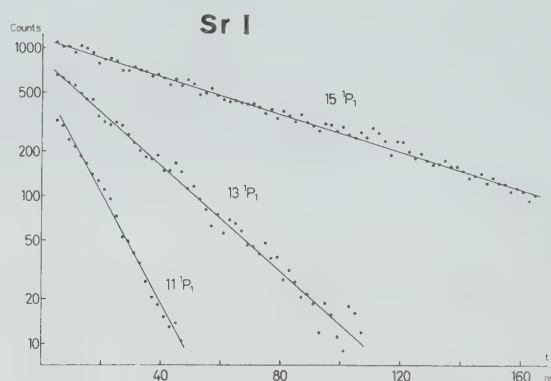


Fig. 3. Three experimental decay curves recorded with a fast transient digitizer. Each curve is the sum of about 500 transients

the metastable $5s4d\ ^1D_2$ state. The subsequent decay was detected on the laser wavelength. Figure 2 shows two experimental PUMOLS-recordings on a logarithmic scale, obtained when the dye laser was running multi-mode. The $5snp\ ^1P_1$ sequence was excited either from the $5s^2\ ^1S_0$ ground state using the pulsed laser system or from the metastable 1D_2 state using pulse-modulated CW light. The decay of 1P_1 states to the $5s4d\ ^1D_2$ state was the easiest to detect but on some occasions the transition to the $5s^2\ ^1S_0$ state was also measured. Figure 3 shows three experimental curves on a logarithmic scale, obtained with the pulsed laser system after adding about 500 transients. Additional measurements of some triplet states was also performed. The excitation then started from the metastable $5s4d\ ^3D$ and $5s5p\ ^3P$ states.

During the lifetime measurements a magnetic field was applied in the excitation volume to avoid influence of slow Zeeman quantum beats. Normal precautions were taken to avoid systematic errors due to multiple scattering or collisions. In the PUMOLS

Table 1. Experimental lifetimes in Sr I. Excitation wavelengths are included

State	Wavelengths [Å]		Lifetimes	
	CW laser system	Excimer laser system	This work [ns]	Other work [ns]
5s 5p ¹ P ₁	4,607			5.12 ^a
5s 6p ¹ P ₁		2,932	65(5)	3.65(14) ⁵
5s 7p ¹ P ₁	5,330	2,569	39.2(20)	4.93(32) ⁵
5s 8p ¹ P ₁	4,481	2,428	27.1(13)	5.46(17) ⁵
5s 9p ¹ P ₁	4,313	2,354	42.7(20)	
5s 10p ¹ P ₁	4,203	2,307	81(6)	
5s 11p ¹ P ₁	4,128	2,275	125(9)	
5s 12p ¹ P ₁	4,076	2,253	170(20)	
5s 13p ¹ P ₁		2,238	250(30)	
5s 14p ¹ P ₁		2,218	510(35)	
5s 15p ¹ P ₁		2,211	690(40)	
5s 16p ¹ P ₁		2,206	925(55)	
5s 17p ¹ P ₁		2,202	1,190(90)	
5s 18p ¹ P ₁		2,199	1,550(120)	
5s 19p ¹ P ₁		2,196	1,890(180)	
5s 20p ¹ P ₁		2,194	2,370(210)	
5s 21p ¹ P ₁		2,192	2,730(260)	
5s 23p ¹ P ₁		2,189	4,270(430)	
5s 25p ¹ P ₁		2,187	5,650(500)	
5s 29p ¹ P ₁		2,184	7,500(900)	
4d 5p ¹ P ₁	4,756	2,429	23.4(23)	
5s 4f ¹ F ₃	5,156		31.3(9)	29.7(9) ⁴ , 33.5(12) ² , 34.2(4) ¹³ , 34.3(28) ¹²
5s 5f ¹ F ₃	4,678		45.0(21)	33.6(13) ² , 53(2) ⁴
5s 6f ¹ F ₃	4,406		78(3)	81(8) ⁴ , 98.5(12) ²
5s 7f ¹ F ₃	4,253		120(5)	133(4) ⁴
5s 8f ¹ F ₃	4,159		179(16)	228(8) ⁴
5s 9f ¹ F ₃	4,096		255(13)	
5s 10f ¹ F ₃	4,052		350(27)	
5s 11f ¹ F ₃	4,021		430(35)	
4d 5p ¹ F ₃	5,598		296(22)	
5s 6s ³ S ₁	7,070		15.0(8)	10.9(11) ¹²
5s 7s ³ S ₁	4,326		34.2(17)	34.8(13) ²
	4,438			
5p ² ³ P ₁	4,742		8.3(4)	8.8(12) ¹² , 10.2(19) ²
	4,784			
	4,876			
5p ² ³ P ₂	4,811		8.3(4)	7.8(12) ¹¹ , 7.89(5) ¹³
5s 5d ³ D ₂	4,872		16.0(6)	16.34(13) ¹³
5s 5d ³ D ₃	4,962		15.9(6)	16.29(24) ¹³ , 17.1(8) ⁴
5s 6d ³ D ₂	4,032		32.0(15)	
5s 6d ³ D ₃	4,030		32.2(16)	34.0(31) ⁴

^a Weighted mean from [5] and references therein

experiments the laser light sometimes had to be attenuated to avoid pile-up in the strong transitions. The time scale corresponding to different TAC ranges were determined using a time delay generator (Berkeley Nucleonics Corp. 7030). The transient digitizer was calibrated with a radio-frequency signal and the channels are separated by 10 ns. The results from our measurements are collected in Table 1. Each state was measured on several occasions. Lifetimes for states measured with both the

laser systems are weighted mean values of all the obtained experimental curves. The lifetime values pertain to room temperature and the influence of black body radiation [7] has not been compensated for. The stated errors include both statistical scattering and estimated possible systematic errors. Included in Table I are also excitation wavelengths [8] and measurements made by other authors. Our lifetime values are in good agreement with literature values, except for the 6–8 ¹P₁ states, previously obtained using the Hanle method [5]. The origin of the large deviations of these lifetime values is unknown*. We also measured the lifetime of the 5s 5p ¹P₁ state. Our result was consistent with earlier established values, but with a larger error due to influence of the excitation pulse.

Discussion

If perturbations are neglected, the radiative lifetimes in a Rydberg series are expected to scale with a power, close to three, of the effective principal quantum number. The 5snf ¹F₃ series, shown in Fig. 4, interacts strongly at n=4 with the doubly excited

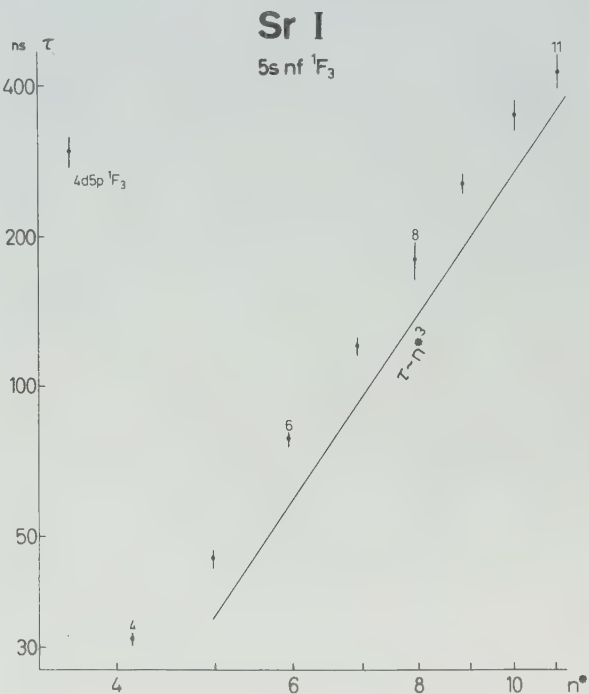


Fig. 4. Experimental lifetimes for the 5snf ¹F₃ (n=4–11) sequence in strontium plotted versus the effective principal quantum number. The diagram is drawn on a log-log scale. The 4d 5p ¹F₃ perturbing state is included. The error bars are indicated by vertical lines. The drawn line indicates the slope in case of an (n*)³ dependence

* Our lifetime values are consistent with results obtained from emission spectroscopy measurements [9]

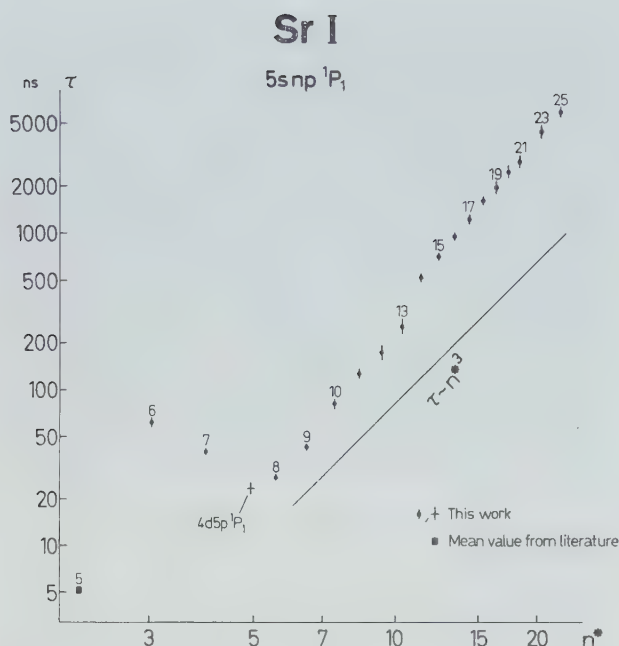


Fig. 5. Experimental lifetimes for the $5snp\ ^1P_1$ ($n=5-25$) sequence in strontium plotted versus the effective principal quantum number. The lifetime value for the $5\ ^1P_1$ state is taken from [5]. The $4d5p\ ^1P_1$ perturbing state is included

state $4d5p\ ^1F_3$. Multiconfigurational Hartree-Fock calculations predict a configuration mixing between the $4d5p\ ^1F_3$ and $5s4f\ ^1F_3$ states close to 50% [10]. A large difference in radiative lifetime between the two states is predicted due to extensive cancellation in the dipole transition from the $4d5p\ ^1F_3$ state to the lowest 1D_2 state. This is in good agreement with our observations. A fit to our experimental data yields $\tau = 0.43(n^*)^{2.91}$ for the rest of the 1F_3 series ($n=5-11$).

The $5snp\ ^1P_1$ series, shown in Fig. 5, is perturbed by the doubly excited $4d5p\ ^1P_1$ state. This state has a shorter lifetime than all the $5snp\ ^1P_1$ states with $n > 5$ and is energy-wise located between the $5s7p$

1P_1 and $5s8p\ ^1P_1$ levels. Calculations based on multichannel quantum defect theory have shown, that the $4d5p\ ^1P_1$ perturber is spread out over a large number of the low-lying 1P_1 states [11]. For lower n -values this interaction may explain most of the deviation from the simple scaling law.

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References

1. Bhatia, K., Grafström, P., Levinson, C., Lundberg, H., Nilsson, L., Svanberg, S.: *Z. Phys. A - Atoms and Nuclei* **303**, 1 (1981)
2. Gornik, W.: *Z. Phys. A - Atoms and Nuclei* **283**, 231 (1977)
3. Grafström, P., Zhan-Kui, J., Jönsson, G., Levinson, C., Lundberg, H., Svanberg, S.: *Phys. Rev. A* **27**, 947 (1983)
4. Osherovich, A.L., Verolainen, Ya.F., Pulkin, S.A., Privalov, V.I., Lupekhin, S.M.: *Opt. Spektrosk.* **46**, 243 (1979) [*Opt. Spectrosc.* **46**, 134 (1979)]
5. Kelly, F.M., Koh, T.K., Mathur, M.S.: *Can. J. Phys.* **52**, 795 (1974)
6. Jönsson, G., Lundberg, H., Svanberg, S.: *Phys. Rev. A* **27**, 2930 (1983)
7. Gallagher, T.F., Cooke, W.E.: *Phys. Rev. Lett.* **42**, 835 (1979); Farley, J., Wing, W.H.: *Phys. Rev. A* **23**, 2397 (1981)
8. Rubbmark, J.R., Borgström, S.A.: *Phys. Scr.* **18**, 196 (1978)
9. Corliss, Ch.H., Bozman, W.R.: *NBS Monograph* 53 (1962)
10. Hansen, J.E., Persson, W.J.: *Phys. B: At. Mol. Phys.* **10**, 363 (1977)
11. Esherrick, P.: *Phys. Rev. A* **15**, 1920 (1977)
12. Brinkmann, U.: *Z. Phys.* **228**, 440 (1969)
13. Andrä, H.J., Plöhn, H.-S., Wittmann, W., Gaupp, A., Stoner, J.O., Gaillard, M.: *J. Opt. Soc. Am.* **65**, 1410 (1975)

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PAPER IX

Experimental and Theoretical Investigation of Radiative Lifetimes in Neutral Gallium

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Using laser spectroscopic techniques the natural radiative lifetimes of $4s^2n_1s^2S$ and $4s^2n_2d^2D$ states of neutral gallium have been measured for $n_1=6$ to 11 and $n_2=4$ to 9. These states, as well as previously measured $4s^2np^2P$ states, have been investigated theoretically using multi-configuration Hartree-Fock calculations. Oscillator strengths to all lower-lying states have been calculated and theoretical lifetimes of the investigated states evaluated. The 2D sequence is strongly influenced by the $4s4p^2^2D$ perturber, and strong cancellation effects in the radiative decay are observed both theoretically and experimentally.

PACS: 31.20.Tz; 31.50.+w; 32.70.Cs

Introduction

During the last few years groups in Lund and Amsterdam have been studying excited states in the group IIIA elements aluminum, gallium and indium. Radiative properties as well as energy substructures have been reported [1–5 and references therein]. By comparing the experimental data obtained using laser spectroscopic techniques, with theoretically obtained data the nature of the different trends and perturbations can often be clarified.

When experimentally investigating the 2D states in Al and In remarkable irregularities in the lifetime trends were found. Previous theoretical studies on the lower 2D states in Al [6, 7] imply that these irregularities are caused primarily by interaction with the sp^2^2D configuration. We expected the same kind of irregularities to occur in the gallium 2D lifetime trend. Earlier calculations of these lifetimes have either

treated only the lowest members of the series [8, 9] or have assumed a single-configuration approach [10]. Previous measurements exist only for some of the lower states and the lifetimes reported show a large variation [10 and references therein]. We therefore considered it valuable to investigate the gallium lifetimes in some greater length and in the present work we present new experimental and theoretical lifetime data for the 2S , 2P and 2D sequences in gallium.

Experimental Set-Up and Measurements

A schematic experimental set-up is shown in Fig. 1. The measurements were performed on an atomic beam of gallium, formed by resistively heating an oven in a vacuum system. As molten gallium is chemically aggressive, forming alloys with low melting points with most refractory metals, the oven was manufactured of boron nitride. In order to avoid multiple scattering and collisions it was essential to keep the density in the atomic beam as low as possible while still maintaining a reasonable signal strength.

Three different laser systems were used to produce

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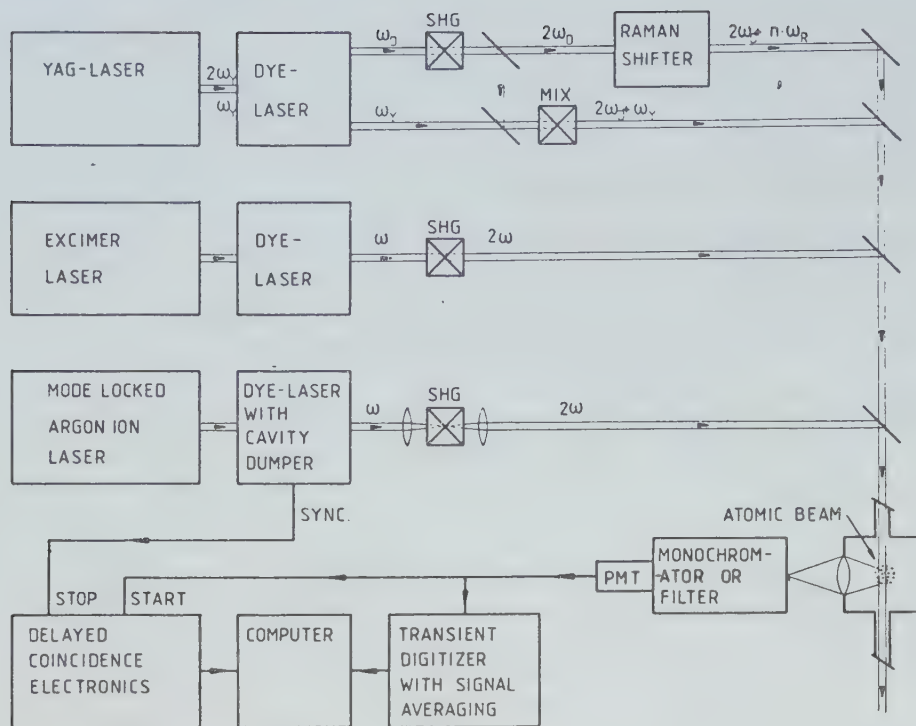


Fig. 1. Schematic experimental set-up showing the three different laser systems used for the lifetime measurements

the light pulses for the measurements. Most of the experiments could be performed with a YAG-pumped (Quanta-Ray DCR-2A) dye laser (Quanta-Ray PDL-1). The pulses from the dye laser, operating on Rhodamine 590, Kiton-red, Sulforhodamine or a mixture of Rhodamine 590 and Kiton-red, were then transferred to UV wavelengths by frequency doubling in a KDP crystal. Still shorter wavelengths required for the higher 2S and 2D states could be produced by frequency mixing of the doubled light with the fundamental (1,064 nm) light from the YAG laser or by using the first, second or third anti-Stokes component from a Raman shifter (Quanta-Ray RS-1, filled with H_2). With frequency mixing a pulse energy of about 2 mJ at 226 nm could be attained. This yield is higher than that which can be obtained using the second anti-Stokes component from the Raman shifter, but the mixing crystal has a cut-off wavelength at ≈ 221 nm, so for the majority of the measurements the more convenient Raman shifter was used for light production. We also tried to Raman shift the mixed light but the overall efficiency was not higher than when using the third anti-Stokes component.

Nearly all of the states were also studied with an excimer-pumped system. An excimer laser (Lambda Physik, EMG-102-E) running on XeCl at 308 nm pumped the dye laser (Lambda Physik, FL-2002) operating on Coumarin 47 or Coumarin 120. The blue laser light was then frequency doubled in

a KPB crystal, at wavelengths down to the cut-off wavelength for KPB at ≈ 217 nm.

The third laser system was used solely when measuring the short-lived $4d\ ^2D$ state. In order to minimize the influence of the shape of the excitation pulse on the fluorescence signal we used a picosecond system for the light production. A mode-locked Ar^+ laser (Coherent Radiation model 468AS mode locker) running at 514 nm gave pulses with a duration of ≈ 120 ps and a mean power of ≈ 1 W that were used to pump the dye laser (Coherent Radiation 599) running on Rhodamine 6G dye. The duration of the pulses from the dye laser was measured with a home-built autocorrelator [11] and the autocorrelation function had a width of 12–14 ps which corresponds to a true width of 8–10 ps. In order to increase the pulse power and decrease the pulse repetition rate (≈ 76 MHz) the dye laser was equipped with a cavity dumper (Coherent Radiation model 7210). With this each pulse made a number (typically 10 or 20) of round trips in the cavity before being dumped. In this way we obtained a mean power of ≈ 60 mW which corresponded to a pulse power of $\approx 1,000$ W. The light from the dye laser was then focused with a 50 mm lens into a KDP crystal giving a conversion efficiency for frequency doubling of the order of 0.5%.

The fluorescence light was detected with a photomultiplier tube (EMI 9558 QB or RCA C31034) through interference- and coloured glass filters or via

a monochromator (Bausch & Lomb, 0.5 m). When measuring the higher 2D states it was necessary to use a monochromator to avoid detecting the light from lower-lying 2S and 2D states. As will be discussed below, the transition probabilities to these lower states (via 2P states) from the high 2D states are large, compared with the transition probability to the ground state. The monochromator was also used when detection was made of the long-wavelength (≈ 750 nm) transitions $nd\ ^2D-5p\ ^2P$. When measuring the $5p\ ^2P$ state we performed the excitation in cascade from the $6s\ ^2S$ state and the detection also in cascade via the $5s\ ^2S$ state. The evaluation was then carried out after a sufficiently long time, so that the influence of the shorter-lived $5s\ ^2S$ and $6s\ ^2S$ states on the decay curve was negligible. To avoid slow Zeeman quantum beats in the fluorescence light, a pair of Helmholtz coils were used to generate a static magnetic field of ≈ 2 mT in the excitation volume. When using the Excimer- or YAG-pumped systems, the transients from the photomultiplier were captured with a transient digitizer (Biomation 8100) equipped with a signal averager for adding transients in order to improve the signal-to-noise ratio. About 2,000 transients were added in each measurement. The data from the signal averager were then sent to a microcomputer for storage and evaluation.

For the long-lived ($\tau > 30$ ns) states the evaluation was made using a standard nonlinear least-squares fit to an exponential plus background. When evaluating the $6s\ ^2S$ state, with a lifetime of ≈ 19 ns, the influence of the finite pulse width (≈ 7 ns) on the signal could not be neglected. In this case the fluorescence curve was fitted with the convolution of a recorded laser pulse and an exponential, with intensity, lifetime, background and the position in time of the laser pulse as free parameters. The same evaluation technique was also tested for the $4d\ ^2D$ state but since the pulse duration and the time between data points in the transient digitizer (10 ns) are of the same magnitude as the lifetime (7.4 ns), the scatter in data was larger than for the $6s\ ^2S$ state and the lifetime could not be determined with satisfactory accuracy.

In order to improve the accuracy the $4d\ ^2D$ state was instead measured with a picosecond system, using delayed coincidence techniques [12]. The signal from the fluorescence photons was amplified in fast pulse amplifiers and sent to a discriminator used in leading-edge trigger mode. To achieve better time resolution, a constant-fraction discriminator could have been used, but the leading-edge trigger was sufficient for this measurement. The output pulse from the discriminator was then used as the start pulse in the time-to-amplitude converter (TAC). The stop pulse was received from the cavity dumper driver via a de-

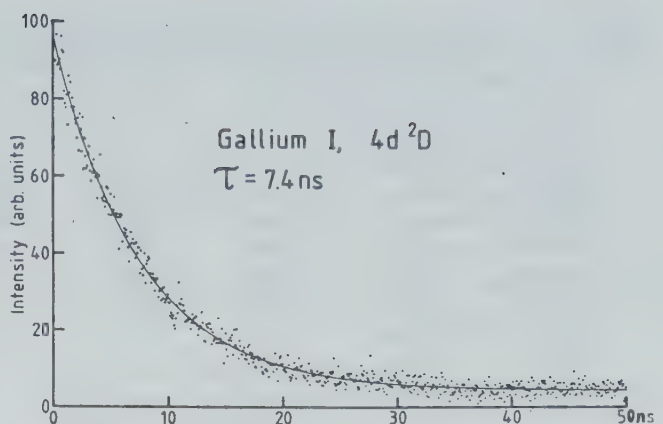


Fig. 2. Experimental decay curve and fitted exponential from the delayed coincidence measurement of the lifetime of Ga $4s^2 4d\ ^2D$

lay generator. The utilization of the photons as start pulses is important in these measurements in order to achieve a high detection efficiency. The TAC has a reset time of more than $2\ \mu\text{s}$ after each start pulse. This means that if the pulse from the dye laser is used as the start pulse, too large a proportion of the fluorescence photons would not be detected due to the high repetition rate of the dye laser (3.8–7.6 MHz). The signal from the TAC was analysed in a multichannel analyser (Tracor Northern, TN-1710) and evaluated in the microcomputer. Pile-up effects were negligible since the number of photons detected per second was only of the order of 500. A decay curve of the $4d\ ^2D$ state is shown in Fig. 2.

Method of Computation

Calculations have been performed for the Rydberg series $4s^2 n_1 s$, $4s^2 n_2 p$, $4s^2 n_3 d$ and $4s^2 n_4 f$, $n_1 = 5$ to 13, $n_2 = 4$ to 12, $n_3 = 4$ to 11 and $n_4 = 4$ to 9.

Wavefunctions were obtained using the MCHF method [13] in a frozen-core approximation, where the $1s$, $2s$, $2p$, $3s$, $3p$ and $3d$ orbitals were taken from a Hartree-Fock calculation of the $4s^2 4p\ ^2P$ state.

The lifetime trend of the $nd\ ^2D$ series depends critically on the decay rate to the $4s^2 4p\ ^2P$ ground state. In the case of the 2D states, the interaction with the $4s 4p\ ^2D$ perturber, lying above the first ionization limit, is such as to produce cancellation in the evaluation of the transition matrix element for the decay to the ground state, making the lifetimes sensitive to the position of the perturber. The J-independent relativistic contributions to the interaction from the Darwin term, mass correction, and spin-spin contact have the effect of lowering the $4s^2 nd$ Rydberg series, having two $4s$ -electrons, relative to the perturber, which has only one.

Table 1. Configurations included in the MCHF calculations

2S	$4s_1^2(^1S)ns_1, 4p_1^2(^1S)ns_1, 4d_1^2(^1S)ns_1, 4f_1^2(^1S)ns_1,$ $5s_1^2(^1S)ns_1, 5p_1^2(^1S)ns_1, 4s_1 4p_1^2(^1S),$ $4s_1 4p_1(^1, ^3P)5p_1, 4s_1 5p_1^2(^1S)$
2P	$4s_1^2(^1S)np_1, 4p_1^2(^1S)np_1, 4d_1^2(^1S, ^3P, ^1D)np_1,$ $4f_1^2(^1S)np_1, 5s_1^2(^1S)np_1, 5p_1^2(^1S)np_1, 4s_1 4d_1(^1, ^3D)4f_2,$ $4s_1 4p_1(^1, ^3P)4d_2, 4p_1^2(^1D)4f_2, 4s_1 5s_1(^1, ^3S)5p_4,$ $4p_1^2(^1S)5p_2$
2D	$4s_1^2(^1S)nd_1, 4p_1^2(^1S)nd_1, 4d_1^2(^1S)nd_1, 4f_1^2(^1S)nd_1,$ $5s_1^2(^1S)nd_1, 5p_1^2(^1S)nd_1, 4s_1 4p_1^2(^1D), 4p_1^2(^3P, ^1D)4d_2,$ $4s_1 4d_1(^1D), 4s_1 4p_1(^1, ^3P)4f_2$
2F	$4s_1^2(^1S)nf_1, 4p_1^2(^1S)nf_1, 4d_1^2(^1S)nf_1, 4f_1^2(^1S)nf_1,$ $5s_1^2(^1S)nf_1, 5p_1^2(^1S)nf_1, 4s_1 4p_1(^1P)4d_2, 4s_1 4p_1(^1P)5g_1$

Table 2. Experimental and theoretical ionization energies in cm⁻¹. The experimental ones are calculated relative to the ionization limit 48,388 cm⁻¹ [17] and the theoretical ones relative to the energy calculated for the ion $(4s^2 4p^2 4d^2 4f^2 5s^2 5p^2)^1S$

	Experiment	MCHF	Experiment -MCHF	Reference for experimental energy level
5s	23,599	22,499	1,100	[16]
6s	10,803	10,495	308	[16]
7s	6,230	6,076	154	[16]
8s	4,056	3,965	91	[16]
9s	2,851	2,795	56	[16]
10s	2,114	2,078	36	[16]
11s	1,630	1,605	25	[16]
12s	1,295	1,277	18	[16]
13s	1,050	1,040	10	This work ^a
4p	47,837	46,999	838	[17]
5p	15,270	14,664	606	[17]
6p	7,984	7,598	386	[17]
7p	4,932	4,734	198	[17]
8p	3,348	3,232	116	[4]
9p	2,428	2,345	83	[18]
10p	1,837	1,777	60	[18]
11p	1,440	1,392	48	[18]
12p	1,159	1,119	40	[18]
4d	13,603	13,564	39	[17]
5d	7,580	7,645	-65	[17]
6d	4,810	4,869	-59	[17]
7d	3,314	3,358	-44	[17]
8d	2,417	2,449	-32	[16]
9d	1,839	1,862	-23	[16]
10d	1,446	1,462	-16	[16]
11d	1,166	1,177	-11	[16]
4f	6,934	6,928	6	[17]
5f	4,433	4,429	4	[17]
6f	3,077	3,072	5	[17]
7f	2,257	2,255	2	[17]
8f	1,727	1,725	2	[17]
9f	1,363	1,362	1	[18]

^a The energy level of 13s was calculated from the laser setting

The sensitivity of the 2D lifetimes to the above relativistic shift effects is reported elsewhere [14]. In that study calculations were performed for the $4s^2 nd^2 D$ series and for the lower members of the

Table 3. Lifetime values for the 2S , 2P and 2D sequences of gallium

State	Lifetime/ns			
	This experiment	Refs. 3 and 4	Corrected for black-body radiation	MCHF ^a
$5s^2 S_{1/2}$				7.2
6	19 (2)		19	18.1
7	49 (5)		49	40.3
8	80 (10)		80	70.3
9	135 (15)		136	111
10	200 (25)		204	169
11	250 (40)		257	247
12				346
13				476
$5p^2 P_{1/2, 3/2}$	55 (5)		55	48.0
$6p^2 P_{1/2}$		172 (9)	172	142
$6p^2 P_{3/2}$		167 (4)	169 ⁷	142
7		380 (20)	384	316
8		660 (40)	690	592
9		920 (60)	1,010	1,007 ¹⁰
10		1,450 (100)	1,700	1,576 ⁸⁰
11		2,000 (200)	2,500	2,335 ⁴⁰
12				3,302 ⁰
$4d^2 D_{3/2, 5/2}$	7.4 (0.3)		7.4	6.8
5	29 (3)		29	24
6	69 (7)		69	74
7	150 (20)		151	169
8	270 (30)		275	282
9	460 (50)		475	400
10				525
11				652

^a The calculations are not J-dependent

$4s^2 np^2 P$ and $4s^2 nf^2 F$ series. The present paper extends the wavefunction calculation to include higher members of the 2P and 2F series and also the $4s^2 ns^2 S$

To be able to keep all the calculations reported in this paper nonrelativistic we recalculated the wavefunctions for the $4s^2 nd^2 D$ series but now without relativistic shifts. The relativistic shifts had however, as mentioned, the important effect of giving the $4s 4p^2 ^2D$ perturber the correct position relative to the $4s^2 nd^2 D$ Rydberg series. To compensate for this we used a slightly different set of configurations, which lowered the Rydberg series relative to the perturber and gave the correct relative position of the perturber. The wavefunctions obtained in this way do not differ appreciably from those reported in [14]. The configurations included are given in Table 1. As in [14] we allow for the inclusion of non-orthogonal orbitals and use the same notation.

The wavefunctions for the $4s^2 ns^2 S$ states were obtained using the configurations listed in Table 1. These calculations caused no convergence difficulties.

To achieve convergence for the higher $np^2 P$

Table 4. Oscillator strengths from lower states to n_1s^2S , $n_1=5$ to 13, n_2p^2P , $n_2=4$ to 12 and n_3d^2D , $n_3=4$ to 11. The oscillator strengths have been calculated using the length formula and experimental transition energies. Those marked unc. are too uncertain to be given but do not give any significant contributions to the total transition probabilities from the upper states

	5s	6s	7s	8s	9s	10s	11s	12s	13s
4p	0.119	0.0155	0.00539	0.00282	0.00172	0.00109	0.000732	0.000515	0.000376
5p		0.315	0.0199	0.00651	0.00316	0.00179	0.00112	0.000757	0.000536
6p			0.468	0.0265	0.00844	0.00397	0.00225	0.00142	0.000962
7p				0.607	0.0336	0.0102	0.00476	0.00269	0.00170
8p					0.733	0.0399	0.0119	0.00551	0.00311
9p						0.880	0.0463	0.0136	0.00628
10p							1.01	0.0522	0.0153
11p								1.14	0.0589
12p									1.34
	5p	6p	7p	8p	9p	10p	11p	12p	
5s	1.35	0.0639	0.0166	0.00696	0.00365	0.00218	0.00142	0.000981	
6s		1.72	0.0930	0.0249	0.0106	0.00564	0.00341	0.00224	
7s			2.10	0.122	0.0332	0.0144	0.00771	0.00470	
8s				2.55	0.143	0.0391	0.0169	0.00907	
9s					2.98	0.164	0.0444	0.0191	
10s						3.42	0.188	0.0512	
11s							3.83	0.213	
12s								4.25	
4d		0.0156	0.00257	0.000890	0.000420	0.000236	0.000147	0.0000983	
5d			0.0210	0.00423	0.00158	0.000782	0.000450	0.000286	
6d				0.0216	0.00489	0.00192	0.000974	0.000570	
7d					0.206	0.00511	0.00208	0.00107	
8d						0.0195	0.00520	0.00217	
9d						unc.	0.0188	0.00529	
10d							unc.	0.0188	
11d								unc.	
	4d	5d	6d	7d	8d	9d	10d	11d	
4p	0.309	0.0426	0.00583	0.00034	0.00008	0.00042	0.00064	0.00073	
5p	0.246	0.558	0.131	0.0472	0.0207	0.0126	0.00753	0.00484	
6p		0.280	0.764	0.165	0.0610	0.0313	0.0178	0.0111	
7p			unc.	1.01	0.194	0.0746	0.0374	0.0217	
8p				unc.	1.12	0.219	0.0844	0.0426	
9p					unc.	1.32	0.245	0.0941	
10p							1.49	0.270	
11p								1.68	
4f			0.0895	0.0105	0.00351	0.00151	0.000856	0.000541	
5f				0.220	0.0259	0.00781	0.00373	0.00212	
6f					0.401	0.0387	0.0131	0.00627	
7f						0.451	0.0553	0.0187	
8f							0.604	0.0721	
9f								0.766	

states, however, a procedure different from the one described in [14] was used. The configurations used are listed in Table 1. The calculations of the excited 2P states were made in two steps. In the first step only configurations not containing any p-orbital outside the core other than np were included and all orbitals outside the core were varied.

In the second step the remaining configurations were included but now only those orbitals not included in the first step were varied. The mp -orbitals, with $m < n$, which in [14] were included to stabilize

np ($n=5$ to 7), but which were not varied, have not been included in these calculations.

The higher members of the $4s^2nf^2F$ series were calculated in the same manner as the lower ones reported in [14].

The wavefunctions were used to determine 2S - 2P , 2P - 2D and 2D - 2F oscillator strengths and transition probabilities using computer programs in the same software package [15] as the MCHF-code. The oscillator strengths were calculated in both the length and the velocity form. Using exact wavefunctions these

values should be identical. If the two forms give identical values, however, there is no guarantee that the wavefunctions are correct. If there, on the other hand, is a large difference between the oscillator strengths obtained with the two different forms this is an indication that some further improvements to the wavefunctions are needed. The radiative lifetimes were finally obtained using the length form of the oscillator strengths. Experimental and theoretical energies of the examined states relative to the ionization limit are given in Table 2. The oscillator strengths and lifetimes were calculated using the experimental transition energies.

Results and Discussion

In Table 3 experimental as well as theoretical lifetimes are presented. To make the Table as complete as possible we have included experimental lifetimes of 2P states from [3] and [4]. In Table 4 the individual theoretical oscillator strengths are presented. For the transitions from the 2D states to the lower 2P and 2F states we used oscillator strengths obtained by using the slightly different, but more stringent, wavefunctions presented as calculation IV in [14]. The difference between these and the ones calculated with the method described here is in all cases very small. Experimental and theoretical lifetimes of the 2S and 2D series are plotted in Figs. 3 and 4. As in Al [2] but unlike in In [1] no significant difference was found between the $J=3/2$ and $J=5/2$ states in the 2D sequence.

When measuring radiative lifetimes the experiment is normally performed at room temperature. This means that there will be a background field due

to black-body radiation present in the measuring volume. This field is very weak at optical frequencies, but as one goes into the infrared region it will increase in strength. Since the frequencies for transitions between different high-lying Rydberg states are often in the infrared region, transitions will be induced by this black-body background field. For long-lived ($> \mu s$) Rydberg states these transitions will clearly influence the measured lifetimes [19]. The measured radiative lifetimes will be shorter than they would have been without the black-body induced transitions. When comparing theoretical and experimental radiative lifetimes of high-lying states it is therefore necessary to, in some way, estimate and correct for this effect. We have made some estimates using formulas and transition rates published by Farley and Wing [20]. In Table 3 one should therefore compare the theoretical lifetime values in column 4 with the corrected values in column 3.

If a Rydberg series is unperturbed the lifetimes increase smoothly as $(n^*)^3$ where n^* is the effective principal quantum number [21]. The converse, however, is not necessarily true. The presence of a perturber might cause deviations from this simple rule, but if the perturber is smeared out over many states the lifetime trend might still appear to scale smoothly. The experimental lifetimes for the $4s^2ns$ and $4s^2np$ series are, after corrections for black-body induced transitions, found to scale close to the ideal $(n^*)^3$ law. The theoretical calculations confirm that they really are "unperturbed". The $4s^2nd^2D$ series however deviates from this rule. The lifetimes do scale smoothly as a power of the effective principal quantum number, but with the power equal to four instead of three. This, however, is accidental. (Compare with

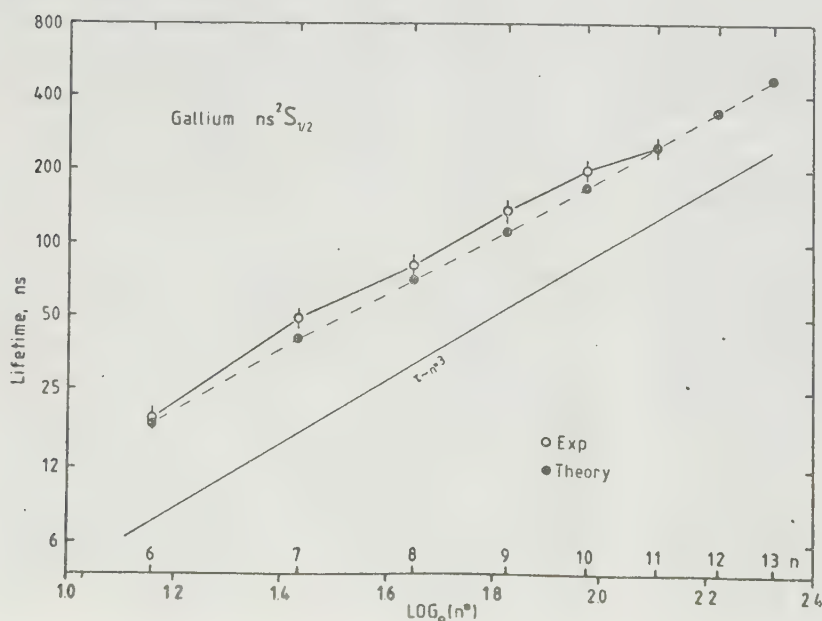


Fig. 3. Experimental and theoretical lifetimes of the $4s^2ns^2S$ states plotted versus the effective principal quantum number

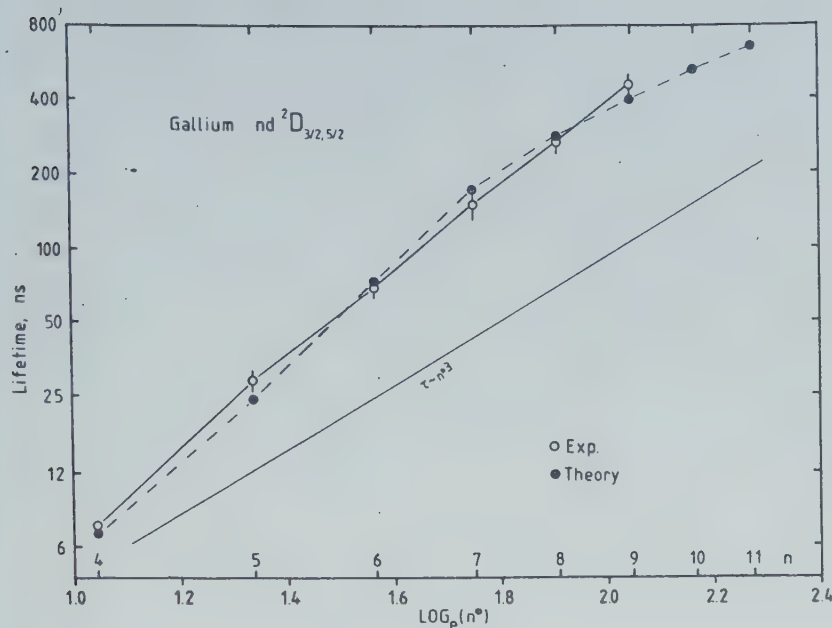


Fig. 4. Experimental and theoretical lifetimes of the $4s^2nd^2D$ states plotted versus the effective principal quantum number

the nd^2D -series in Al and In where the same kind of perturbation exists, [1] and [2].) The theoretical calculations clearly demonstrate how strongly perturbed this series is. The mixing between the $4s4p^2^2D$ perturber and the $4s^2nd^2D$ states gives two different contributions to the transition matrix elements between the ground state and each of the 2D states. These two contributions have different signs and different n -dependencies resulting in strong cancellation for $n=7$ to 10. This can be observed by studying the individual transitions to the ground state (Table 4). When the measurements were performed on the 2D states one could clearly observe this cancellation effect. After selectively populating the $8d$ or $9d$ states much stronger fluorescence light was detected for transitions to the excited $5p$ state, where no cancellation occurs, than for transitions to the ground state. The detailed theoretical study of the interaction between the $4s^2nd$ Rydberg series and the $4s4p^2$ perturber is published elsewhere [14].

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References

- Jönsson, G., Lundberg, H. Svanberg, S.: Phys. Rev. A **27**, 2930, (1983)
- Jönsson, G., Lundberg, H.: Z. Phys. A - Atoms and Nuclei **313**, 151 (1983)
- Jönsson, G., Levinson, C., Svanberg, S., Wahlström C.G.: Phys. Lett. **93A**, 121 (1983)
- Jönsson, G., Levinson, C., Lindgren, I., Persson, A., Wahlström, C.G.: Z. Phys. A - Atoms and Nuclei **322**, 351 (1985)
- Zaki Ewiss, M.A., Snoek, C., Dönszelmann, A.: Astron. Astrophys. **121**, 327 (1983)
- Weiss, A.W.: Phys. Rev. A **9**, 1524 (1974)
- Froese Fischer, C.: Phys. Scr. **23**, 38 (1981)
- Migdalek, J., Baylis, W.E.: J. Phys. B **12**, 2595 (1979)
- Aashamar, K., Luke, T.M., Talman, J.D.: Phys. B **16**, 2695 (1983)
- Lindgård, A., Mannervik, S., Jelenkovic, B., Veje, E.: Z. Phys. A - Atoms and Nuclei **301**, 1 (1981)
- Carlsson, J., Rüter, F.: Lund Reports on Atomic Physics, **51** (1985)
- Demtröder, W.: Laser spectroscopy V. In: Springer Series in Optical Sciences. Vol. 30, Ch. 11. Berlin, Heidelberg, New York: Springer 1981
- Froese Fischer, C.: The Hartree-Fock method for atoms. New York: Wiley 1977
- Brage, T., Froese Fischer, C., Carlsson, J., Wahlström, C.-G.: Submitted for publication.
- Froese Fischer, C.: US Department of Energy report No. DOE/ER/10618-11 (1983)
- Moore, C.E.: Atomic Energy Levels, Vol. II, NSRDS-NBS 35, Washington, D.C. 1971
- Johansson, I., Litzen, U.: Ark. Fys. **34**, 573 (1967)
- Young, W.A., Mirza, M.Y., Duley, W.W.: Opt. Commun. **34**, 353 (1980)
- Gallagher, T.F., Cooke, W.E.: Phys. Rev. Lett. **42**, 835 (1979)
- Farley, J.W., Wing, W.H.: Phys. Rev. A **23**, 2397 (1981)
- Bethe, H.A., Salpeter, E.E.: Quantum mechanics of one- and two-electron atoms. New York: Plenum 1977

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PAPER X

Lifetimes and oscillator strength trends for the $4s^2nd\ ^2D$ series of Ga I.

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Theoretical transition probabilities for $kf\text{-}nd$ and $mp\text{-}nd$ transitions in Ga I, ($k = 4$ to 6 , $m = 4$ to 7 , and $n = 4$ to 8) are reported together with lifetimes for the first five members of the $4s^2nd\ ^2D$ series. Mixing with $4s4p^2\ ^2D$ is found to be very important. The sensitivity of the $nd\ ^2D$ lifetimes to the position of this perturber is discussed, together with the oscillator strength trend for the transitions from the $nd\ ^2D$ series, $n = 4$ to 11 , to the ground state. The calculated lifetimes are in good agreement with recent laser experiments.

PACS numbers: 31.20.Tz, 31.50.+w, 32.70.Cs and 32.70.Fw

1. INTRODUCTION

Recent measurements of the lifetimes in Ga I of levels in the $4s^2nd\ ^2D$ series, using laser techniques,¹ show a strong divergence from the normal $(n^*)^3$ trend, where n^* is the effective principal quantum number.

Previous studies of the homologous Al I sequence² suggests that these irregularities are caused primarily by the interaction with the $4s4p^2\ ^2D$ configuration. Such $sd-p^2$ interactions are known to be strong from studies of other systems, e.g. Mg-I-like ions³. We therefore expect that this configuration will have a large influence on the diffuse series, even though it has an energy about 5000 cm^{-1} above the ionization limit* (to be compared with a binding energy of about 13000 cm^{-1} for the $4d$ electron in $4s^24d\ ^2D$.) This implies that even though Ga I is essentially a one-electron system, with normal terms of the form $4s^2nl\ ^2L$, the "softness" of the $4s$ shell introduces correlation between the $4s$ and nl electrons.

Earlier calculations on the 2D series either have treated only the lowest member^{5,6} or have assumed a single-configuration approach.⁷ For higher n values, semiempirical quantum-defect theory has been used to deduce the position of the perturber.⁸

From a theoretical point of view it can be argued that a perturber imbedded in the continuum should give rise to a Beutler-Fano profile⁹ in the transition probabilities, which can be extrapolated into the discrete Rydberg series. We also know from photoabsorption studies that the $msmp^2\ ^2D$ state, in group III atoms, gives rise to a very broad resonance, and has been suggested to cause a minimum in transition probabilities around $n=9$ for Ga I and In I ($m = 4$ and 5 respectively).¹⁰

This minimum, which results from a cancellation effect (see below), causes the lifetimes of the 2D states to be very sensitive to the contributions from transitions to the excited 2P and 2F states. Thus, to obtain reliable lifetimes of the higher 2D states, a large number of states have to be included in the calculation.

In this paper we consider

- a) lifetimes for $4s^2nd\ ^2D$, $n = 4$ to 8 ,
and
- b) the oscillator strength trend for the $4s^24p\ ^2P-4s^2nd\ ^2D$ transitions,
 $n = 4$ to 11 .

II. METHOD OF CALCULATION

Wavefunctions were obtained using the Multiconfiguration Hartree-Fock (MCHF) package¹¹ in a frozen-core approximation, where the $1s$, $2s$, $2p$, $3s$, $3p$ and $3d$ -orbitals were taken from a Hartree-Fock calculation of the ground state, $4s^24p\ ^2P$. The wavefunction expansion for each state are summarized in Table I, where only orbitals with the same indices are orthogonal, and the orbitals without indices are orthogonal to all one-electron functions with the same orbital quantum number l . For example, $4p_1$ and $5p_1$ are orthogonal, and so are $3d$ and $4d_1$, but not $4d_1$ and $4d_2$. Test calculations have shown that the core polarization has only a limited effect on the transition probabilities and therefore is not included in the final calculations.

i) p states

To get convergence for the $np\ ^2P$ states, we had to change the expansion in going from the ground state to the excited states by including some lower-lying configuration states of the same symmetry. In the calculations for the 5p state we included $4s, ^24p_1$, as obtained from a Hartree-Fock calculation of the ground state, without optimizing the corresponding $4p_1$ orbital during the MCHF procedure. In the calculations for 6p, $4p_2, ^2(^1S)5p_2$ was included, together with the lower $4s, ^24p_2, ^2$ and $4s, ^25p_2$ configuration states. In the optimization of this state the $4p_2$ and $5p_2$ orbitals were kept fixed. Since test calculations showed that the np orbitals were very similar in $4s^2np$ and $4p^2(^1S)np$, the same orbital, labelled np_2 , was used in both cases for the higher states ($n = 6$ and 7). Calculations for the 7p state were performed in a similar manner as for the 6p state (see Table I). Instead of calculating the 8p state, an extrapolation of the probabilities for np - nd transitions was used to obtain a value for the $4s^28p\ ^2p - 4s^28d\ ^2D$ transition probability.

ii) d states

Since the 2D states were much more stable than the 2P -states, no lower members of the Rydberg series had to be included. Because of the cancellation in the transition probability, it is very important to get a good representation of the perturber. According to Fano⁹, the "unperturbed" position of $4s4p^2\ ^2D$ can be observed as the "midpoint" of an absorption resonance in the continuum. That is, the energy distance between our full MCHF calculation for the $nd\ ^2D$ states and the perturber, without the interactions with the d-series included, should agree with experimentally obtained energy differences between the bound 2D -states and the position of the resonance profile for $4s4p^2\ ^2D$. To test how sensitive our results were to the agreement in energy differences between theory and experiment, we performed four different types of calculations (I-IV below).

Since the inclusion of extra correlation within the $4s^2$ shell only affects the Rydberg states, and not the perturber, we tested two different representations. First, including the complex of $4s^2$, we used the set

$$(4s^2 + 4p^2 + 4d^2 + 4f^2)^1S$$

in calculations I and III. Then, in calculations II and IV the $5s^2$ configuration was also included in the representation of the 1S core. A consistent approach for calculation of transition energies demands that the same representation be used for the "core" in both the initial and final state, thus an additional configuration had to be included in all states.

Similarly, relativistic effects contribute to the energy of the 2D series and the perturber in different ways. The Darwin term, mass correction, and spin-spin-contact term, which are J-independent contributions to the energy matrix, mainly affect the s electrons. Therefore they will contribute more to the energies of the $4s^2nd$ configurations than to $4s4p^2$, which has only one occupied 4s orbital. In calculation III these relativistic effects are included as perturbations, after the optimization of the orbitals, in calculation I. In the same way calculation IV represents an inclusion of these effects in calculation II. Table II describes the different types of calculations schematically.

Since we have to find a finite expansion for each 2D state, the important question is: How do we select the right configurations to include? The mixing between the $4s^2nd$ series and $4s4p^2$ 2D results in a cancellation in the transition matrix element around $n = 8$, thus the lifetimes of these states are very sensitive to small changes in the contributions to the oscillator strengths. Hence, it is not sufficient only to consider the magnitude of the mixing coefficients in the MCHF representation of the Rydberg states, and reject all configurations with small weights. Some configurations with small weights may be important in determining the position of the perturber. Since the weight of the perturber will depend strongly on a good representation of its correlations, a separate calculation was performed for $4s4p^2$ 2D , without including the s^2nd -states. The energy of this "unperturbed" state should correspond to the position of the observed absorption resonance in the continuum, as discussed above.

III. DISCUSSION AND RESULTS

In an unperturbed Rydberg series the lifetimes increase smoothly as $(n^*)^3$, but the presence of a perturber may cause an irregular behavior. The mixing between the perturber and the $4s^2nd$ 2D states results in two different contributions to the transition matrix element between the ground state and the d-states. The transition element is given, approximately, by the expression

$$\begin{aligned} \langle 4s^24p \ ^2P | E1 | 4s^2nd \ ^2D \rangle &= c_1 \langle 4s^24p \ ^2P | E1 | 4s^2nd \ ^2D \rangle \\ &+ c_2 \langle 4s^24p \ ^2P | E1 | 4s4p^2 \ ^2D \rangle \end{aligned} \quad (1)$$

These two contributions have opposite signs and different n -dependence. In the first, the transition integral decreases with increasing n because of the decreasing overlap between the $4p$ and the nd wavefunctions. In the second, the c_2 coefficient can be written approximately as

$$c_2 = \langle 4s^2nd \ ^2D | V | 4s4p^2 \ ^2D \rangle / \Delta E_n \quad (2)$$

Where ΔE_n is the energy difference between the perturber and the nd Rydberg state. Analogous to the integral in the first term, the absolute value of the numerator decreases with increasing n , because of the decreasing overlap between the $4p^2$ and the $4snd$ pairs, but since the perturber is situated above the entire Rydberg series, ΔE_n also will decrease. This causes the absolute value of the first term in (1) to decrease faster than the second, as can be seen in Table III. Their different signs will therefore give rise to a pronounced cancellation for some value of n . For high n the Rydberg states are very closely spaced, so the numerator decreases faster than the denominator and the second term will eventually start to decrease also (see Table III). From Table III it is also obvious that the single configuration approach, used in Ref. 7, is not valid for higher 2D states since it does not take the effect of the perturber into account. The different calculations predict different relative positions of the perturber and the Rydberg states, and thereby also different positions for the minimum in transition probabilities. The separations, which are listed in Table IV.

increase in going from calculation I to calculation IV, with the experimental value of Kozlov and Startzev⁴ being between that of III and IV. The value derived from the semi-empirical quantum defect theory by Neijzen and Dönszelmann⁸ is slightly above that of calculation IV.

After the minimum, which is equivalent to the minimum in the Beutler-Fano profile of $4s4p^2\ ^2D$, the total probability for the $4s^24p\ ^2P - 4s^2nd\ ^2D$ transition will increase. The contribution to the matrix element in (1) from the second term will dominate as the first decreases. Because of the broadness of the resonance profile the exact position of the perturber is not known, but Kozlov and Startzev give a wavelength of 1860 Å for the multiplet $4s^24p\ ^2P - 4s4p^2\ ^2D$. The energy differences between the $4s^2nd\ ^2D$ states and the perturber derived from this wavelength are given in Table IV under observed. As a crude estimate of the uncertainties in this value for the excitation energy of the perturber, the separation between the two lines $4s^24p\ ^2P_{1/2} - 4s4p^2\ ^2D_{3/2}$ and $^2P_{3/2} - ^2D_{5/2}$ may be used. This separation is given by the differences in fine structure splitting of the two terms involved. For $4s4p^2\ ^2D$ Neijzen and Dönszelmann⁸ derive $E(5/2 - 3/2) \approx 165\text{ cm}^{-1}$ and for the ground state we have¹⁵ $E(3/2 - 1/2) = 826\text{ cm}^{-1}$. From this the separation between the two lines is $d \approx 660\text{ cm}^{-1}$. In Fig. 1 the experimental position of the perturber is shown with these estimated errors. In Table IV, the oscillator strengths for the $4s^24p\ ^2P - 4s^2nd\ ^2D$ transitions are listed, together with the different methods. The inclusion of J-independent relativistic effects are seen to lower the energy of the Rydberg states more than the energy of the perturber, thereby increasing the distance between them. The inclusion of the $5s^2nd\ ^2D$ configuration states will depress the Rydberg series similarly, but this represents a much smaller effect. In Fig. 1, the trends for $f_e = f(n^*)^3$, the effective oscillator strength¹², are shown for calculations I and III. It is obvious from these curves that relativistic effects lower the energy of the Rydberg states, increase the $4s^24d - 4s4p^2$ distance, and shift the position of the oscillator strength minimum towards higher n-values. A comparison of the four calculations shows how sensitive the resulting transition properties are to a good representation of the $4s4p^2\ ^2D$ state.

For transitions to 2F and excited 2P states the contribution from the second term in (1) is zero since the transition to these states from $4s4p^2\ ^2D$ is forbidden. The mixing of $nd\ ^2D$ states with the perturber, therefore, will affect only the c_1 -coefficient in the expression

$$\langle 4s^2mp\ ^2P | E1 | "4s^2nd" ^2D \rangle = c_1 * \langle 4s^2mp\ ^2P | E1 | 4s^2nd \rangle ^2D; m > 4 \quad (3)$$

In table V the A values for all transitions contributing to the lifetimes of the 2D -states, together with the corresponding transition energies, are reported. The calculated lifetimes, obtained by method III and IV, confirm the most recent experimental results,¹ especially for states with energy close to the minimum ($n = 6$ to 8). The theoretical transition probability for the $8p\ ^2P - 8d\ ^2D$ transition was estimated from an extrapolation of probabilities for $np-nd$ ($n = 4$ to 7) transitions. When this estimate is included in calculation IV, the calculated lifetimes for the most critical states, $n = 6-8$, are within the error bars of the experimental results (see Table VI). More important, the results reported here follow the same trend along the sequence as experiment, while the single configuration approach⁷

breaks down for $n > 4$.

IV. CONCLUSION

In this paper we have shown that the $4s4p^2 \ ^2D$ perturber has a pronounced effect on the probabilities for transitions from the ground state to members of the $4s^2$ nd Rydberg series, and even causes an almost complete cancellation for $n = 7-9$.

The different types of calculations, which give different positions for the perturber relative to the Rydberg series, demonstrate the sensitivity of the oscillator strengths to a "correct" representation of an important perturber. Therefore in calculations of lifetimes, this type of perturber, and its associated correlation, has to be included in an accurate manner.

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REFERENCES

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Nashville, TN 37235, USA.
1. J. Carlsson, H. Lundberg, W.X. Peng, A. Persson, C.-G. Wahlström,
T. Brage and C. Froese Fischer, accepted for publication in Z. Phys.D.
 2. C. Froese Fischer, Phys. Scr. 23, 38 (1981).
 3. C. Froese Fischer and M. Godefroid, Nucl. Instr. Methods 202, 307
(1982).
 4. M.G. Kozlov and G.P. Startzev, Optics and Spectrosc. 24, 3 (1968).
 5. K. Aashamar, T.M. Luke and J.D. Talman, J. Phys. B16, 2695 (1983).
 6. J. Migdalek and W.E. Baylis, J. Phys. B12, 2595 (1979).
 7. A. Lindgård, S. Mannervik, B. Jelenkovic and E. Veje, Z. Phys. A301,
1 (1981).
 8. J.H.M. Neijzen and A. Dönszelmann, Physica 114C, 399 (1982).
 9. U. Fano, Phys. Rev. 6, 1866 (1961).
 10. J.P. Connerade and M.A. Baig, J. Phys. B14, 29 (1981).
 11. C. Froese Fischer, DOE Report No. Doe/ER/10618-11 (1983).
 12. K.T. Cheng and C. Froese Fischer, Phys. Rev. A28, 2811 (1983).
 13. I. Johansson and U. Litzén, Arkiv för fysik 34, 573 (1967).
 14. G. Jönsson, C. Levinson, I. Lindgren, A. Persson and
C.-G. Wahlström, Z. Phys. A322, 351, (1985).
 15. C. Moore, Atomic Energy Levels, NSRDS-NBS 35, Vol. II, U.S.
Government Printing Office, Washington, D.C. 20402.

TABLE I. Wavefunction expansions.

In all calculations the core is represented as $1s^2 2s^2 2p^6 3s^2 3p^6 3d^{10}$

A. $4s^2 np^2 P$

Part 1. n-dependent basis set

i. $(4s_1^2 + 4d_1^2 + 4f_1^2)(^1S)np_1^2 P$

ii. $4p_2^2(^3P, ^1D, ^1S)np_2^2 P$

n=4: ii. is replaced by $4p_2^3^2 P + 4p_2^2(^1S)5p_2^2 P$ and $4d_1^2(^3P, ^1P)4p_1^2 P$

is added.

n=6,7: np_1 is replaced by np_2 .

Part 2. common to all

iii. $4s_1 5s_1(^3S, ^1S)4p_3^2 + 4p_2^2(^1D)4f_2^2 P + 4s_1 4p_3(^3P, ^1P)4d_2^2 P +$
 $+ 4s_1 4d_3(^3D, ^1D)4f_2^2 P$

Part 3. lower state of same symmetry

n=5: $4s_1^2 4p_1^2 P$

n=6: $4s_1^2 np_2^2 P$ for n=4,5

$4p_2^2 5p_2^2 P$

n=7: $4s_1^2 np_2^2 P$ for n=4 to 6

$4p_2^2 np_2^2 P$ for n=5,6

B. $4s^2 nd^2 {}^2D$

$$\begin{aligned}
 & (4s_1^2 + 4p_1^2 + 4d_1^{2*} + 4f_1^2)({}^1S)nd_1^2 {}^2D + 4s_1 5s_1 ({}^3S, {}^1S)nd_2^2 {}^2D + \\
 & + 4s_2 (4p_2^2 + 4d_2^2 + 4f_3^2)({}^1D) {}^2D + 4p_2 5p_2 ({}^3D)4s_2^2 {}^2D + \\
 & + 4p_3 4f_2 ({}^3D, {}^1D)4s_2^2 {}^2D + 4p_4 4d_4 ({}^3F, {}^3D, {}^3P, {}^1F, {}^1D, {}^1P)4f_4^2 {}^2D + \\
 & + 4p_2^2 ({}^3P, {}^1D)4d_5^2 {}^2D
 \end{aligned}$$

* in $4s^2 4d^2 {}^2D$ we have used $4d_6^3 {}^2D + 4d_6^2 5d_6^2 {}^2D$

C. $4s^2 nf^2 {}^2F$

$$\begin{aligned}
 & (4s_1^2 + 4p_1^2 + 4d_1^2 + 4f_1^{2*})({}^1S)nf_1^2 {}^2F + 4s_2 4p_2 ({}^3P, {}^1P)4d_2^2 {}^2F + \\
 & + 4s_2 4d_3 ({}^3D, {}^1D)4f_2^2 {}^2F
 \end{aligned}$$

* in $4s^2 4f^2 {}^2F$ we have used $5f_1^2 ({}^1S)4f_1^2 {}^2F$

D. $4s4p^2 {}^2D$

all configurations after $4s_2 4p_2^2 {}^2D$ in B.

TABLE II. Schematic description of the different types of calculations.

Calculations	Relativistic effects included	$5s^2nl$ included
I	No	No
II	No	Yes
III	Yes	No
IV	Yes	Yes

TABLE III. Contribution to the $\langle 4s^2 4p \ ^2P | E1 | 4s^2 nd \ ^2D \rangle$ matrix element. From calculation IV (see Text).

n	$c_1 \langle 4s^2 4p \ ^2P E1 4s^2 nd \rangle$	$c_2 \langle 4s^2 4p \ ^2P E1 4s 4p^2 \rangle$	Total $S^{1/2}$
4	3.5652	-0.6040	3.0009
5	1.6196	-0.6137	1.0223
6	0.9079	-0.5509	0.3658
7	0.5584	-0.4791	0.0865
8	0.3665	-0.4137	-0.0405
9	0.2507	-0.3518	-0.0956
10	0.1832	-0.3051	-0.1168
11	0.1324	-0.2614	-0.1246

TABLE IV. Observed and calculated distances between the perturber, $4s4p^2\ ^2D$ and the $4s^2nd\ ^2D$ states, and oscillator strengths for $4s^24p\ ^2P - 4s^2nd\ ^2D$ transitions. In each group the first entry is the energy distance, in cm^{-1} the second the oscillator strength in length form and the third the oscillator strength in velocity form.

n	Calculations				Others ^a	
	I	II	III	IV	Ref. 4	Ref. 8
4	17131	17317	18916	19148	18980 ^b	19420 ^b
	0.280	0.284	0.299	0.301		
	0.279	0.279	0.300	0.302		
5	11083	11273	12926	13174	12950 ^b	13400 ^b
	0.0313	0.0336	0.0393	0.0413		
	0.0315	0.0328	0.0409	0.0424		
6	8278	8476	10104	10334	10180 ^b	10630 ^b
	0.0017	0.0024	0.0047	0.0057		
	0.0018	0.0024	0.0057	0.0067		
7	6751	6954	8599	8827	8690 ^b	9140 ^b
	0.00038	0.00010	0.00010	0.00033		
	0.00029	0.00008	0.00035	0.00067		
8	5829	6037	7694	7915	7790 ^c	8240 ^c
	0.0021	0.0013	0.00027	0.00007		
	0.0019	0.0012	0.00006	0.00000		
9	5232	5442	7112	7336	7210 ^c	7660 ^c
	0.0031	0.0022	0.00075	0.00047		

	0.0028	0.0020	0.00035	0.00016		
10	4824	5037	6715	6938	6820 ^c	7270 ^c
	0.0032	0.0025	0.00098	0.00063		
	0.0029	0.0023	0.00053	0.00032		
11	4533	4748	6430	6658	6540 ^c	6990 ^c
	0.0032	0.0024	0.00103	0.00072		
	0.0030	0.0023	0.0062	0.00040		

^a Energy of the perturber from experiment (ref. 4) and semi empirical quantum defect theory (ref. 8).

^b Energies of nd states from ref. 13.

^c Energies of nd states from ref. 15.

TABLE V. Transition energies, in cm^{-1} , (observed and calculated) and transition probabilities, in s^{-1} , for $4s^2 4p \ ^2P - 4s^2 nd \ ^2D$. (Only transition probabilities contributing more than 1% to the lifetime for a d-state or with $A > 10^4$ are listed). Calculated transition probabilities are scaled with experimental transition energies. In each group the first and second entries are experimental and theoretical excitation energies respectively and the third and fourth give transition probability from method III and IV (see text).

upper lower	4d ^a	5d ^a	6d ^a	7d ^a	8d ^c	9d ^c	10d ^c	11d ^c
4s ² 4p ² P ^a	34235 33197 1.45(8) 1.46(8)	40257 39186 2.62(7) 2.76(7)	43028 42009 3.56(6) 4.32(6)	44523 43514 8.44(4) 2.67(5)	45420 44419 2.28(5) 6.24(4)	45998 45000 6.49(5) 3.60(5)	46391 45397 8.67(5) 5.52(5)	46671 45682 9.18(5) 6.39(5)
4s ² 5p ² P ^a	1667 1136 2.73(5) 2.74(5)	7690 7126 1.30(7) 1.32(7)	10460 9948 5.61(6) 5.74(6)	11956 11453 2.58(6) 2.70(6)	12853 12358 1.27(6) 1.37(6)			
4s ² 6p ² P ^a		404 77 1.68(4) 1.83(4)	3174 2899 3.01(6) 3.08(6)	4670 4404 1.42(6) 1.44(6)	5567 5309 7.39(5) 7.57(5)			
4s ² 7p ² P ^a				1618 1421 1.05(6) 1.06(6)	2515 2326 4.88(5) 4.91(5)			
4s ² 8p ² P ^b					931 --- 5.23(5) ^d 5.23(5)			
4s ² 4f ² F ^a			2124 2044 3.51(5) 3.77(5)	3620 3549 1.32(5) 1.28(5)	4517 4454 6.79(4) 6.69(4)			
4s ² 5f ² F ^a				1119 1066 2.73(5) 2.57(5)	2016 1971 1.00(5) 9.83(4)			
4s ² 6f ² F ^a					658 622 1.74(5) 1.62(5)			

^a Ref. 13

^b Ref. 14

^c Ref. 15

^d Obtained by extrapolation of probabilities for the $np \ ^2P - nd \ ^2D$ transition, $n = 4$ to 7.

TABLES VI. Lifetimes for $4s^2nd^2D$ states in nanoseconds.

nd=	4d	5d	6d	7d	8d
Calculated					
I ^a	7.36	29.7	100.1	180	220 ^b
II ^a	7.25	28.3	92.1	182	224 ^b
III ^a	6.88	25.5	79.7	180	278 ^b
IV ^a	6.82	24.5	74.2	169	282 ^b
Observed					
Ref. 1	7.4±0.3	29±3	69±7	150±20	270±30
Other					
Calculated					
Ref. 5	6.90 ^c				
Ref. 6	6.27 ^c				
Ref. 7 j=1/2	7.08	12.7	24.1	41.5	80.7
j=3/2	7.20	13.0	24.7	42.7	82.6
Observed					
Ref. 7 j=1/2	5.8±0.6	16±2	32±3		
j=3/2	5.8±0.6	15±2	32±3		

^a Calculations reported here (see text).

^b Includes transition probability for $8p^2P - 8d^2D$ extrapolated from the trend of $np^2P - nd^2D$ transition probabilities (n=4 to 7).

^c Transition to $5p^2P$ not included.

Figure Captions

Fig. 1 Effective oscillator strengths for the $4s^24p\ ^2P - 4s^2nd\ ^2D$ transitions as a function of the energy of the nd states relative to 4d.

- Nonrelativistic, calculations I. *
- Relativistic, calculations III. **

Also indicated is the position of the perturber, $4s4p^2\ ^2D$, as obtained from

- a. Nonrelativistic calculation I.*
- b. Relativistic calculation III. **
- c. Kozlov and Startzev⁴
- d. Neijzen and Dönszelmann⁸

* See text.

** Including relativistic shifts, see text.

